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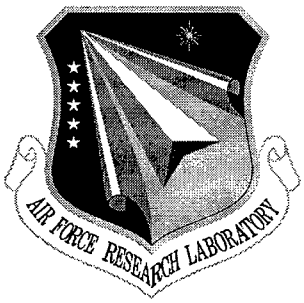

QUANTUM MECHANICS OF COMPUTING IN CONDENSED MATTER SYSTEMS

Clarkson University

Vladimir Privman, and Lawrence S. Schulman

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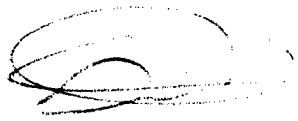

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13. ABSTRACT *(Maximum 200 words)*

New conceptual models for solid state fermionic interactions have been investigated for quantum computational atomic-level systems. The effects of decoherence in general as well as adiabatic decoherence upon coherent states of quantum computational elemental structures have been analyzed. Hamiltonians for quantum mechanical logic gates have been derived. The main result has been a new proposal for quantum computation in solid-state systems in the regime of the quantum Hall effect. These results provide insight into the quantum mechanical issues facing the new field of quantum information theory.

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1.0 PROGRESS REPORT

1.1 Research Work Carried Out and Future Directions

Recently, two proposals have been formulated theoretically for realizations of quantum computing which can be potentially done in solid-state systems. They utilize, respectively, quantum-dots and nuclear-spins, the latter in the quantum-Hall effect (QHE) regime. The possibility of quantum computing in solid-state devices is exciting. Indeed, the intricacies of modern technology, especially as far as nanoscale "engineering" is concerned, are much more geared for solid-state systems than any other medium. All modern electronic devices, with, presently, components on submicron scales, are solid-state.

However, unlike the more "established" quantum computing proposals such as ion traps and liquid-state NMR, the two solid-state proposals, both several-month old, are presently theoretical. The PI of this project, V. Privman, is a co-author of the original proposal for quantum-Hall quantum computing. The appended research article, Section 2.0, details this research work. As future work, there are several theoretical investigations needed, of the form and strength of the spin-spin interactions, of the time scales of interaction vs. decoherence, and other topics, before initial experimental attempts to build few-qubit systems can be deemed realistic. These will be surveyed later in this section.

Our research results have also included studies of the XOR and controlled-NOT gates. We derived explicit quantum Hamiltonians for these gates; see Section 3.0. We have also addressed the nature of decoherence in quantum computing. We have initiated a project to consider spin interactions with bosonic and multispin heat baths, to supplement recent results by Ekert's group. The latter effort is detailed in Section 4.0. Any quantum computer will necessarily make contact with the external environment and in general such interactions cause entanglement of the computer's degrees freedom with those of the environment. We investigated whether this inevitably led to decoherence. This work is summarized in Section 5.0.

Future work will invlude elucudation of the form of the spin-spin interactions for the quantum-Hall quantum computer. Terms in the effective phenomenological two-spin interaction Hamiltonian have been tentatively identified in the recent literature based on the second-order perturbative calculation, carried out for two identical nuclei. Such a calculation must be carried out to include estimation of interaction parameters, and for dissimilar nuclei. The quantities to be determined are the precise form of all the terms in the interaction Hamiltonian of two spins as well as the strength of the interaction.

Even more importantly, there are methods in the density-matrix perturbative approach that allow calculation of the coherence time T_2 during which the system avoids decoherence. These techniques require perturbative expansions not much more complicated that the interaction energy calculations. However, to our knowledge, they were never utilized in the field of quantum computing. It will be of great interest to apply these techniques, not only for the QHE quantum computer but also in the quantum-dot and possibly liquid-state NMR versions.

On the subject of decoherence, future work will focus on models where both decoherence and thermalization can be studied analytically. The results can then be used to gauge the validity of the density-matrix perturbative techniques mentioned in the preceding paragraph.

Many of the techniques needed for interaction control in the QHE system can be adopted from the liquid-state NMR formulation. However, we would like to develop means to switch interactions on and off at will, for varying time intervals. Switching on a pair-wise interaction would allow to carry out a unitary transformation on a pair of spins independently of the other spins. It has been established that nearly any such transformation, combined with single-spin transformations which can be accomplished by radiation pulses, form a universal set. We plan to study effects of placing impurities between nearest-neighbor spins, which can be ionized by external electromagnetic pulses to electronic configurations that capture electrons and locally destroy the coherence of the electron gas, thus decreasing the spin-spin interactions. Differentiation can be achieved by using different impurity species.

The process of "feeding in" the initial data into the computer need also be further investigated. One proposal has been to shine polarized light at the system that creates electron-hole pairs. These pairs annihilate, forcing on a fixed nuclear spin polarization, corresponding to that of the incident light. After the initial alignment, the nuclear spins can be rotated to the desired quantum states needed for computation by electromagnetic pulses at their respective frequencies.

Reading off the final spin states by measuring requires further study. As for the liquid-NMR proposal, we could read off averages by producing replicas of the spin chain and letting them evolve in parallel. The electromagnetic pulses that control the computation can be applied to all the replicas at once. It is plausible to assume that the final state is one of the direct-product states of the n-spin system. It is possible to generate by holographic and other methods a narrow strip of conductance at each spin in turn and send a current of spin-polarized electrons through it. The observed current can be pre-calibrated to enable high certainty determination of whether there was a spin-

exchange scattering event thus determining the nuclear spin's direction, resembling the spin-diode techniques. Furthermore, one can have several replicas of the spin chain, separated order of magnitude more than the spins, e.g., ~1000 Å. One can probably have enough of them to **reduce** significantly any uncertainty in the spin direction determination. Feasibility of these as well as some other ideas based on the Aharonov-Bohm effect must be explored.

1.2 Publications

The following articles will be published presenting the results of this project:

Design of Gates for Quantum Computation: the Three-Spin XOR in Terms of Two-Spin Interactions, D. Mozyrsky, V. Privman and S. P. Hotaling, *Int. J. Modern Phys.* B (1998), in print.

Invited Review. Hamiltonians for Quantum Computing, V. Privman, D. Mozyrsky and S. P. Hotaling, in the Proceedings of the Conference *Photonic Quantum Computing. AeroSense 97* (SPIE—The International Society for Optical Engineering, 1997), SPIE Proceedings Vol. 3076, 84-96.

Invited Review. Lower Bounds for Decoherence, L. S. Schulman, in the Proceedings of the Conference *Photonic Quantum Computing. AeroSense 97* (SPIE—The International Society for Optical Engineering, 1997), SPIE Proceedings Vol. 3076, 76-82.

Bounds on Decoherence and Error, L. S. Schulman, *Phys. Rev. A* **57**(2) (1998), in print.

Continuous and Pulsed Observations in the Quantum Zeno Effect, L. S. Schulman, *Phys. Rev. A* (1998), in print.

Quantum Computation in Quantum-Hall Systems, V. Privman, I. D. Vagner and G. Kventsel, *Phys. Lett.* A (1998), in print.

Adiabatic Decoherence, D. Mozyrsky and V. Privman, *J. Statist. Phys.* (1998), in print.

1.3 Presentations and Student Participation

The following presentations have resulted from this project:

Presentations by V. Privman

"Hamiltonians for Quantum Computing" — Condensed Matter Workshop Seminar at Beer-Sheva University, Israel, January 6, 1997.

"Hamiltonians for Quantum Computing" — Colloquium at Technion, Haifa, Israel, January 9, 1997.

"Hamiltonians for Quantum Computing" — Invited Talk at SPIE conference Photonic Quantum Computing, April 23, 1997; also Session Chair for "Quantum Computer Design Issues."

"Analog Quantum Computation and Statistical Mechanics" — Talk at 77th Statistical Mechanics Meeting, Rutgers University, May 19, 1997.

"Hamiltonians for Quantum Computing" — Invited Talk at First Killam Workshop on Quantum Information Theory, University of Montreal, Canada, May 29, 1997.

"Hamiltonians for Quantum Computing" — Colloquium at MPIF/CNRS Hochfeld-Magnetlabor, Grenoble, France, June 19, 1997.

"Hamiltonians for Quantum Computing" — Colloquium at University of Nancy, France, July 11, 1997.

"Hamiltonians for Quantum Computing" — Colloquium at University of Mainz, Germany, July 17, 1997.

"Quantum Computing" — CNLS Seminar at Los Alamos National Laboratory, August 8, 1997.

"Quantum Computation: Getting Closer to Reality" — Invited Talk at the DIMACS Quantum Computing Workshop, Princeton University, August 14, 1997.

"Quantum Computing" — Condensed Matter Seminar at University of Pittsburgh, November 6, 1997.

"Quantum Computing" — Condensed Matter Seminar at University of Rochester, November 24, 1997.

1997 Presentations by L. S. Schulman

1/31 Tulane Univ., New Orleans, "How Quick is a Quantum Jump."

2/13 Univ South Carolina, Columbia, "Time's Arrows and quantum measurement."

4/23 Conf.: Photonic Q. Comp., Orlando, "Lower Bounds on Decoherence."

5/22 Charles University, Prague, "The quantum Zeno effect."

6/23 Univ. Rome I, Rome, "Quantum Zeno effect."

6/25 IROE (Microwave res. inst.), Florence, "Observing and preventing quantum jumps."

6/26 Univ. Florence, Arcetri, "Time's Arrows Quantum Measurement."

8/21 Conf. Non-equilib. stat. mech., Michigan, "Time symmetric thermodynamics: theoretical & observational (plenary lecture)."

10/8 Univ. Rochester, Rochester, "Time's Arrows and Quantum Measurement."

11/27 Institute Henri Poincaré, Paris, "Week of Path Integral Lectures, at "Borel Symposium" Three mathematical challenges in path integration."

12/12 Clarkson Univ., Potsdam, "How quick is a quantum jump?."

Presentation by D. Mozyrsky (graduate student)

"Models of Adiabatic Decoherence" — Invited Talk at the DIMACS Quantum Computing Workshop, Princeton University, August 14, 1997.

The above colloquium/seminar presentations were attended largely by graduate students, and some undergraduates. One of the coauthors of the papers listed, Mr. Mozyrsky, is a graduate student at Clarkson University. Two other graduate students. Ms. Folger and Mr. Park, recently begun working on this project at Clarkson. Furthermore, two undergraduate students have worked with V. Privman on a wider field of Physics of Nanoscale Devices, as their Summer '97 projects (paid for by Clarkson).

2.0 RESEARCH ARTICLE

Quantum Computation in Quantum-Hall Systems

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Abstract

We describe a quantum information processor (quantum computer) based on the hyperfine interactions between the conduction electrons and nuclear spins embedded in a two-dimensional electron system in the quantum-Hall regime. Nuclear spins can be controlled individually by electromagnetic pulses. Their interactions, which are of the spin-exchange type, can be possibly switched on and off pair-wise dynamically, for nearest neighbors, by controlling impurities. We also propose the way to feed in the initial data and explore ideas for reading off the final results.

The field of quantum computing has seen an explosive growth of theoretical development [1-7]. It has been realized that quantum computers can be faster than classical computers for some problems [1-3,8-13]. The analog nature of errors and possible error correction schemes have been explored [6,7,9,13-21]. There have also been several proposals for actual realizations of quantum information processing [4,5,13,22-31]. Two of these proposals: the ion-trap system [5,22,25,27,28] and the ensemble-of-molecules liquid-state NMR approach [29-31] have been studied extensively as possible experimental realizations of quantum computing. However, all experimental results to date only accomplish the simplest quantum-logic functions such as single-spin rotations or two-spin controlled-NOT [1-7].

A major challenge faced by both experiment and theory has involved scaling up from one to many quantum gates and actual "programming," i.e., conducting calculations by coherent quantum unitary evolution, in a controlled fashion. Experimentally, quantum computation requires switching on and off pair-wise interactions between various two-state systems, e.g., spins $\frac{1}{2}$, termed "qubits." Initialization and reading off the final results are also nontrivial parts of the process. Ideally, the latter should involve efficient measurement of a single qubit. The NMR variant [29-31] measures instead ensemble averages (expectation values). Certain "fault-tolerant" error correction schemes [7,13,17,19-21] actually also require measurements of some of the qubits *during* the computation.

Theoretically, the most striking recent development has been the formulation of the fault-tolerant error correction schemes [7,13,17,19-21]. Correction of analog errors inherent in quantum computation due to the superposition-of-states property (which in turn is central to the speed-up of some calculations) means an uphill battle against the second law of thermodynamics. These error-correction schemes [7,13,17,19-21] aim at calculations that can go on indefinitely provided the overall error rate at each qubit is small enough.

It is not our goal here to review these issues: we will adopt the point of view that modern error correction schemes will allow calculations long enough to be useful provided a working quantum information processor can be devised. It is the latter aspect that we address in this work. Thus, we propose a quantum computer realization based on hyperfine interactions [32] between the conduction electrons and nuclear spins embedded in a two-dimensional electron system in which the electron gas is in the quantum-Hall effect (QHE) regime [33,34]. Such systems have been made at the interfaces

between semiconductor materials and in superlattices (layered semiconductor structures) [35].

In these systems, at temperatures of order 1K and applied magnetic fields of several Tesla, there are intervals of magnetic field values for which the electrons fill up an integer number of Landau levels [36]. The electron gas then forms a nondissipative QHE fluid [35]; the Hall resistance exhibits a plateau at a value that is a multiple of e^2/h, while the dissipativity of the conduction electron gas (the magnetoresistance) approaches zero. Nuclear-spin thermalization/relaxation processes occur on the time scale denoted T_1 [32] which, experimentally, ranges from several minutes to half an hour [37-39]. It is expected then that the nuclear spin dynamics is dominated by coherent spin exchanges mediated by electrons [40,41]. Owing to rapid advances in the experimental facilities, the hyperfine interactions in QHE systems have recently attracted growing theoretical [41,42] and experimental [37-39] interest; this progress makes it feasible to handle the electron spin-nuclear spin interactions with almost atomic precision.

Similar to the ion-trap system [5,22,25,27,28], we consider a chain of spin-$\frac{1}{2}$ nuclei, of atoms positioned by the molecular-beam epitaxy techniques [35] in an effectively two-dimensional system subjected to a strong magnetic field. The typical separation should be comparable to the magnetic length $\ell_H = \sqrt{\hbar c/eH}$, where H is the applied magnetic field, perpendicular to the two-dimensional layer. This length is of the order of 100 Å. We propose to control individual nuclear spins by electromagnetic-radiation pulses in the nuclear magnetic resonance (NMR) frequency range [32].

An important question is how to control nuclear spins individually. Use of magnetic field gradient could be contemplated to achieve differentiation, but there are severe limitations on the field variation owing to the need to maintain the QHE electronic state. Instead, one can use *different nuclei*. Theoretically, there is no apparent limit on how many different spins can be arranged in a chain. However, practically the number of suitable spin-$\frac{1}{2}$ isotopes may be limited. Thus, achieving sufficient chemical-shift dispersion for systems of more than few qubits may require additional ideas; the following ones are tentative because presently it is not known how realistic these proposals are from the point of view of actual experimental realizations. Specifically, one can position nuclear spins in different crystalline environments. The latter can be controlled by implanting atoms and complexes into

the host material [32]. It may be also possible to utilize small clusters of nuclear spins, rather than individual spins. These can be made coherent [43] by lowering the temperature to order several μK, as compared to order 1K needed to achieve the QHE state.

Under the typical conditions of QHE the direct dipole-dipole interaction of the nuclear spins is negligibly small [41]. The dominant interaction will be that mediated by the contact hyperfine interactions between nuclear spins and conduction electrons [40]. Similarly, electron-mediated interactions leading to the scalar coupling have been utilized in the liquid-state NMR realization of quantum computation [29-31]. In ordinary metals, the electron-mediated nuclear-spin interactions exhibit Friedel oscillations [32] because of the existence of sharp Fermi surface.

In the quantum-Hall regime, however, the energy spectrum of the two-dimensional electron gas is discretized by the magnetic field. As a result, the interaction is no longer oscillatory but rather monotonic, exponentially decaying [40] on the length scale ℓ_H. The following terms in the effective phenomenological two-spin interaction Hamiltonian correspond to the second-order perturbative calculation (carried out for two identical nuclei) of [40], where for different nuclei we replaced Z^2 by the product of the two atomic numbers (which is basically a guess),

$$-VZ^{(1)}Z^{(2)}H^{-1}\sqrt{\frac{c\ell_H}{r}}e^{-cr/\ell_H}\left[\sigma_-^{(1)}\sigma_+^{(2)}+\sigma_+^{(1)}\sigma_-^{(2)}\right], \qquad (1)$$

where c is a dimensionless quantity [40] of order 1, $Z^{(j)}$ are the atomic numbers of the nuclei, while V is some constant. Note that

$$r/\ell_H \propto r\sqrt{H}\,. \qquad (2)$$

Here H is the applied field, r is the spin-spin separation, while $\sigma^{(j)}$ are the Pauli matrices corresponding to the spin-$\frac{1}{2}$ operators of the two nuclei labeled by the superscripts $j=1,2$. Each nuclear spin also interacts with the applied field via the magnetic coupling of the form $-\gamma^{(j)}\hbar H\sigma_z^{(j)}$. Determination of the precise effective spin-spin interaction Hamiltonian will likely to be accomplished to a large extent by direct experimental probe. The strength of the interaction in Eq. (1) can be roughly estimated to be of order 10^{-16} erg, which corresponds to frequency of order 10^{11} Hz.

For quantum computation, one has to devise the means to control the spin-spin interactions. Ideally, one would like to be able to switch interactions on and off at will, for varying time intervals Δt. Switching on a pair-wise interaction would allow to carry out a unitary transformation on a pair of spins independently of the other spins. It has been established [13,23,44-47] that nearly any such transformation, combined with single-spin transformations which can be accomplished by radiation pulses, form a universal set in the sense that arbitrary "computer program" can be built from them. There are NMR "refocusing" methods that allow such control, as utilized, for instance, in the liquid-state NMR formulation [29-31] of quantum computing. However, until the full form of the spin-spin interaction Hamiltonian is established for our case, it is useful to consider other ideas as well.

Geometry constraints would limit the pairs of spins for which the two-spin interactions are nonnegligible typically to nearest-neighbor pairs. Furthermore, other interactions cannot be really *fully* eliminated, but only reduced. Still, control of the spin-spin interactions would allow added flexibility in "programming" the unitary evolution of a computational device. Even when the control is possible, in practice it would be unrealistic to expect the form of the interaction, such as Eq. (1) above, be known exactly from theoretical calculations alone. Thus, Eq. (1) is a leading-approximation/guess phenomenological form. Input from experiments will be required to fine-tune the computer functions that depend on such internal interactions.

One possibility not based on the NMR methods is to disrupt (ideally, switch off), for the duration of some time interval Δt, the interaction for one (nearest-neighbor) pair of spins by placing impurities between the spins, see Figure 1. The impurities can be ionized by external electromagnetic pulses to electronic configurations that capture electrons and locally destroy the coherence of the electron gas. Differentiation can be achieved by using different impurity species. Admittedly, this is a rather speculative idea. Specifically, it may be more appropriate to place the impurities near or surrounding the nuclear spins, instead of the geometry of Figure 1.

It is important to emphasize that the pair-wise interactions are "on" most of the time, for each pair of spins. Therefore, the "idle" unitary transformations in the latter approach will not be simple phase changes as for noninteracting spins. The ability to change the interactions locally, pair-wise, will only allow to change the *relative* unitary transformations to which nearest-neighbor spin pairs are subject. In addition, one has the single-spin rotations

that can be done by external electromagnetic pulses. Programming of such a computer is therefore less straightforward than usually expected in the theoretical approaches that assume *noninteracting* idling elements [1-7,13,23,44-47]; however, this is only a matter of new mathematical developments being called for.

We now turn to the process of "feeding in" the initial data into the computer. This can be accomplished as follows: initially, all the nuclear spins in the system are pumped in one direction. This can be achieved by shining a polarized light at the system [49] that creates electron-hole pairs. These pairs annihilate, forcing on a fixed nuclear spin polarization, corresponding to that of the incident light [49]. After the initial alignment, the nuclear spins can be rotated to the desired quantum states needed for computation by electromagnetic pulses at their respective frequencies.

In all the proposals for quantum computation [1-7,13,22-31], reading off the final spin states by measuring, and also the measurement processes that are required for error correction [7,13,17,19-21], are most challenging to realize. This is because direct interaction of a microscopic system with any macroscopic system for the purpose of measurement is disruptive and difficult to carry out in an orderly fashion for all the individual spins in the system.

We note that as for the liquid-NMR proposal [29-31], we could read off averages by NMR techniques by producing replicas of the spin chain, see Figure 1, and letting them evolve in parallel. The electromagnetic pulses that control the computation can be applied to all the replicas at once. However, some quantum error correction protocols [7,13,17,19-21] require actual measurements rather than averages. Furthermore, unlike the liquid-state NMR, there may be uncontrollable differences between the replicas. The only thing that might save the situation is the fact that our spins are located at distances much larger than atomic dimensions. Therefore, some averaging of the "atomic" scale influences may be expected in the spin-spin interactions controlling the actual computation in each chain. The latter observation suggests that measurement methods other than NMR-based must be explored. We propose three measuring processes below: the first and second may be more appropriate for final-state readout while the second and third for error-correction schemes.

First, let us assume that the final state is one of the direct-product states of the n-spin system. It is possible to generate by holographic and other

methods [48-51] a narrow strip of conductance at each spin in turn, see Figure 1, and send a current of spin-polarized electrons through it. The observed current can be pre-calibrated to enable high certainty determination of whether there was a spin-exchange scattering event thus determining the nuclear spin's direction, resembling the spin-diode [38,52] techniques. Furthermore, one can extend the strip of conductance over several replicas of the spin chain, separated order of magnitude more than the spins, e.g., 1000 Å. One can probably have enough of them to reduce significantly any uncertainty in the spin direction determination.

Second, if the final or intermediate state (the latter case is relevant for error correction) can be entangled, so that one cannot simply measure each spin in turn, then the situation is more complicated. One can generate a "mask" of conducting strips, for all or a group of spins. However, "calibration" to derive data pertinent to the multispin quantum state may be a challenge.

Third, some error correction schemes [7,13,17,19-21] require measurement of difference of the components of nearby spins. This might be contemplated by having two conducting strips with the spin-polarized electron current, and adding a time-dependent component to the applied magnetic field for the duration of the measurement. Difference in the nuclear spin states will then affect the Aharonov-Bohm oscillatory structure of the observed current; see [53] for survey of such effects.

In summary, we have proposed a model of a quantum computer based on the hyperfine interactions between the electron and nuclear spins in quantum Hall effect systems. This brings to two the number of proposals that have been formulated theoretically for realizations of quantum computing which can be potentially done in *solid-state systems*; the other is the quantum-dot proposal [26]. The possibility of quantum computing in solid-state is exciting. Indeed, the intricacies of modern technology, especially as far as nanoscale "engineering" is concerned, are much more geared for solid-state systems than any other medium. All modern electronic devices, with, presently, components on submicron scales, are solid-state.

However, unlike the more "established" quantum computing proposals such as ion traps and liquid-state NMR, the two solid-state proposals are presently theoretical. There are several investigations needed, of the form and strength of the spin-spin interactions, of the time scales of interaction vs. decoherence, and other topics, before initial experimental attempts to

build few-qubit QHE quantum-computing systems can be deemed realistic. Specifically, no estimates are available of the time scales of decoherence which may be orders of magnitude shorter than T_1.

We wish to thank D. Mozyrsky for helpful comments on the manuscript and P. Wyder for the hospitality at Grenoble HFML and interest in this work. The work of V.P. has been supported in part by US Air Force grants, contract numbers F30602-96-1-0276 and F30602-97-2-0089. I.V. acknowledges support by a grant from the German-Israeli Foundation for Scientific Research and Development, number G 0456-220.07/95.

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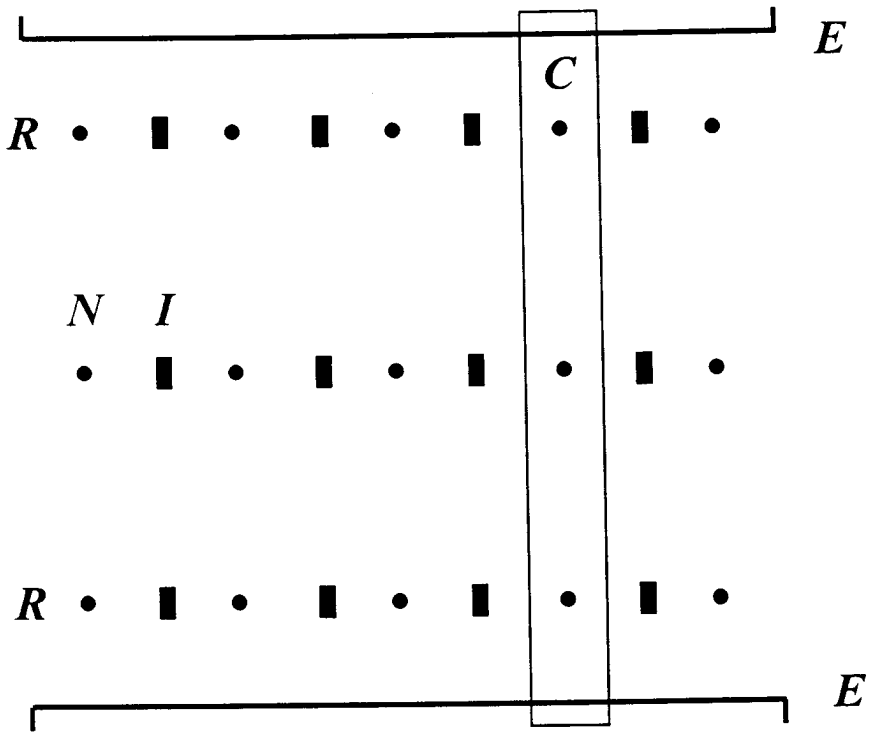

Figure 1: The schematics of the proposed two-dimensional nuclear-spin system: N denotes atoms with spin-$\frac{1}{2}$ nuclei; I denotes impurity atoms or complexes that can be ionized to disrupt the spin-exchange interactions mediated by conduction electrons (the impurity placement may be different, see text); R illustrate replicas (actually there will be many of them); E and C represent conducting electrodes and connecting strip for measurement (see text).

3.0 RESEARCH ARTICLE

Hamiltonians for Quantum Computing

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ABSTRACT

We argue that the analog nature of quantum computing makes the usual design approach of constructing complicated logical operations from many simple gates inappropriate. Instead, we propose to design multi-spin quantum gates in which the input and output two-state systems (spins) are not necessarily identical. We outline the design criteria for such devices and then review recent results for single-unit Hamiltonians that accomplish the NOT and XOR functions.

Keywords: Quantum computing, Analog computing, Hamiltonians for quantum gates

1. INTRODUCTION

One of the great challenges of the physics of nanoscale systems has been the design of atomic-size devices operating in a quantum-coherent fashion. Dimensions of semiconductor computer components will soon reach[1] about $0.25\,\mu\mathrm{m} = 2500\,\text{Å}$, which is well above the atomic sizes at which quantum-mechanical effects are important. However, it is generally expected that as the miniaturization continues, atomic dimensions will be reached. This article concerns with quantum computing, i.e., nanoscale devices that perform logical operations while maintaining quantum coherence. Some early studies[2-4,8,9] considered how quantum mechanics affects the foundations of computer science: issues such as limitations on classical computation due to quantum fluctuations, etc., have been raised. A more recent development[4-32] has been to utilize the quantum nature of components of atomic dimensions for more efficient computations involving quantum-coherent evolution.

Quantum computing has attracted a lot of interest recently owing to several new features. Firstly, it may be faster than classical computing: new fast quantum algorithms have been proposed.[33-37] Error correction techniques,[10,27,33,38-42] unitary operations corresponding to the simplest logic gates,[5-32] and some Hamiltonians for gate operation[10,11,14,24,28-32,43] have been explored. Ideas on how to combine the simplest quantum gates have been put forth.[7,15,44] Experimentally, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized[26,45,46] or contemplated.[19]

There remain, however, many conceptual difficulties with quantum computing.[4,18] The reversibility of coherent quantum evolution implies that the time scale Δt of the operation of quantum logic gates must be built into the Hamiltonian. As a result, all the proposals available to date assume that computation will be externally timed, i.e., interactions will be switched *on* and *off*, for instance, by laser radiation.

This means that if logical operations are constructed from one or few simple universal gates, then each such gate will have to be precisely controlled from outside. In ordinary classical (i.e., macroscopic, irreversible) computing, the NAND gate is an example of a universal gate. From it complicated logical operations can be constructed. In the classical case, however, it is the internal relaxation processes in the basic gate(s) that determine the time scale of their operation (equilibration) Δt. We consider it extremely unlikely that one would ever be able to control externally, in a coordinated fashion, millions of simple reversible quantum gates in order to operate a macroscopic computer.

Furthermore, quantum computers are naturally *analog*[22] in their operation. Indeed, in order to use the power of quantum interference (superposition of states), one has to allow any linear combination of the basis qubit states $|1\rangle$ and $|0\rangle$. Analog errors are difficult to correct. By analog errors we mean those minor variations in the input

and output variables which cannot on their own be identified as erroneous in an analog device because its operation involves *continuous* values of variables (so that the fluctuated values are as legal as the original ones). By noise errors we term those that result from single-event problems with device operation, or from external influences (including decoherence in the quantum case), or from other failures in operation. All errors in a *digital* device (i.e., deviations from discrete values) can be systematically decreased or eliminated in each step of a calculation. Similarly, the noise errors in analog devices can be corrected or decreased.

However, the analog errors cannot be corrected. Consider a state $\alpha|1\rangle + \beta|0\rangle$ and a nearby state $\alpha'|1\rangle + \beta'|0\rangle + \sum_j \zeta_j|j\rangle$, where α' is close to α, β' is close to β, while ζ_j are small. The latter terms represent admixture of quantum states $|j\rangle$ other than the two qubit states. Both states are equally legal as input and output quantum states. We could restrict input or output to a vicinity of certain states, for instance, the basis states $|1\rangle$ and $|0\rangle$, thus moving towards digitalization. However, we then loose the quantum-interference property. Another important effect: decoherence, that would require a density matrix description, falls in the noise-error category.

Modern error-correction techniques[10,27,33,38-42] can handle the noise errors but not the analog errors. To illustrate, consider this quote[42] from the article entitled *Quantum Error Correction for Communication*: "To achieve this the sender can add two qubits, initially both in state $|0\rangle$, to the original qubit and then perform an encoding unitary transformation...". The problem here is that the states actually encountered in the system during error correction are not available as basis qubit states (such as $|0\rangle$) with infinite precision. Typically, by qubits we mean a set of two orthogonal quantum states selected from the energy eigenstates of the system. Even assuming that the thermal noise can be reduced at low temperatures to make the ground state sufficiently long-lived, the excited states of any system, especially if it is a part of a macroscopic computer, will not be defined sharply enough to provide ideal stationary states $|1\rangle$ and $|0\rangle$. External interactions, spontaneous emissions, etc., will generate both noise- and analog-errors in the basis states, i.e., the actual state (disregarding decoherence) will be $\alpha|1\rangle + \beta|0\rangle + \sum_j \zeta_j|j\rangle$, with $\alpha \simeq 1$ and $\beta, \zeta_j \simeq 0$, instead of the ideal $|1\rangle$ which is an eigenstate of an ideal, isolated-system Hamiltonian.

Furthermore, analog errors will be magnified when separate simple-gate operations are combined to yield a complex logical function. Thus, the conventional picture of a quantum computer is unrealistic: it assumes a multitude of simple-gate units each being externally controlled by laser beams (one needs a lot of graduate students for that!). Such computers will magnify analog errors which cannot be corrected in principle because the error state is as legal as the original state.

In this work we therefore adopt a view typical of the analog-computer approach, of designing the computer as a single unit performing in one shot a complex logical task instead of a chain of simple gate tasks. This approach will not repair all the ailments outlined earlier. For instance, the computer as a whole will still be subject to analog errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a sufficiently large time interval to function as parts of a larger classical (dissipative) computer which will not maintain a quantum-coherent operation over its macroscopic dimensions. We would like these to function as single analog units rather then being composed of many gates.

The outline of this review is as follows. In Section 2 we continue our discussion of the design of quantum gates. In Section 3 we review known results for the simplest NOT gate mainly to set the notation and nomenclature. A more complicated, two-spin NOT gate is studied in Section 4. Section 5 addresses the time-dependence of the Hamiltonians. Finally, Sections 6, 7, 8 review results for a three-spin XOR gate.

2. DESIGN CONSIDERATIONS FOR MULTI-SPIN QUANTUM GATES

In order to make connections with the classical computer-circuitry design and identify, at least initially, which multi-qubit systems are of interest, we propose to consider spatially extended multi-spin quantum gates with input and output qubits possibly different. The reason for emphasizing this property is that multi-spin devices will have spatial extent. The interactions that feed the input need not be identical to those interactions/measurements that read off the output. Furthermore, for systems with short-range interactions one can only access the boundary spins in a large cluster. Thus we may use only part of the spins to specify the input and another subset to contain the output. The two sets may be identical, partially overlapping, or nonoverlapping.

Reversibility of coherent quantum evolution makes the distinction between the input and output less important than in irreversible computer components. However, we consider the notion of separate (or at least not necessarily fully identical) input and output useful within our general goals: to learn what kind of interactions are involved and to consider also units that might be connected to/as in classical (dissipative) computer devices.

Our goal is to be able to design interaction parameters, presumably by numerical simulations, to have such gates perform useful Boolean operations. This is not an easy task. Actually, it must be broken into several steps. First, we must identify those interactions which can be realized in solid state or other experimental arrangements. As examples below illustrate for several simplest gates the form of the interaction Hamiltonians is quite unusual by the solid-state standards.

Secondly, we expect interactions to be short-range and two-particle (two-spin) when several two-state systems (termed qubits, spins) are involved.

Thirdly, incorporating designed coherent computational units in a larger classical computer will require a whole new branch of computer engineering because the built-in Boolean functions will be complicated as compared to the conventional NOT, AND, OR, NAND, etc., to which computer designers are accustomed. Furthermore, the rules of their interconnection with each other and with the rest of the classical computer will be different from today's devices.

Our initial studies have been analytical. In the future we foresee numerical studies of systems of order 20 to 25 two-state (spin) atomic components with variable general-parameter interactions. In this review we summarize results[28,31,32] for interaction Hamiltonians required for operation of the NOT (Sections 3,4) and XOR (Sections 6, 7, 8) logic gates. Other results presently available include Hamiltonians for certain NOT[14,28] and controlled-NOT gates,[10,30,43] and for some copying processes,[29,30] as well as general analyses of possibility of construction of quantum computing systems.[8,22]

Quantum logics and the dynamics of quantum gates should be fully reversible. Implications of this property have biased recent literature on the quantum logic gates. Firstly, the distinction between the input and the output parts of the system has been blurred. A typical configuration involves a quantum-mechanical system that is "programmed" with the input and then after the time interval Δt it will be in the output state. We note that the time interval Δt is fully determined by the parameters of the Hamiltonian; in order to effect the quantum gate operation, the interaction energies associated with both the internal and external-field parts of the Hamiltonian must be of order $h/\Delta t$.

Consideration of multi-spin quantum gates requires a large number of basis states. However, it is also useful to study few-spin exactly solvable systems. These provide explicit examples of what the actual interaction Hamiltonians should look like. A notable exactly solvable system, known before the quantum-computing field became active, is the NOT gate operation in a two-state qubit[14] obtained by applying a constant external magnetic field to a single spin. Then another field is applied, oscillating in time, in a direction perpendicular to the constant field. This *paramagnetic resonance* problem is a textbook example of time-dependent quantum-mechanical evolution.

An accepted approach has been to consider interactions switched on only for the duration of the gate operation Δt. If the gate is actually the whole computer then one can regard the interaction as time-independent. However, for specific tasks in components with a limited number of basis states, it may be appropriate to view the interaction as controlled externally to be switched on and off. While general ideas of externally timed computation are not new,[4] actual realizations in quantum computation with many sub-unit gates will encounter difficulties outlined earlier. General developments for the latter type of interaction (time-independent or on/off) have included[8,22] identification of unitary operators that correspond to quantum computer operation and establishment of the existence of the appropriate interaction Hamiltonians.

A quantum gate performs an operation whereby the input state determines the output state after a time interval Δt. The interactions must be controlled, i.e., switched on and off, in order to have the gate operation during the interval Δt independent of the interactions with the computer parts external to the gate. This control of interaction, i.e., external timing of the computer operation already mentioned earlier, can be possibly accomplished by the external interactions while the internal interactions be reserved for the gate operation. However, we would like to consider multi-spin gates in order to avoid too many such controlling external influences.

With regards to the requirement to control the interactions externally, with the time dependence given by the on/off protocol, we will show in Section 5 how to extend this approach to certain time-dependent interactions (protocols) which are more smooth than the on/off shape.

3. THE SIMPLEST NOT GATE

In this section we consider the NOT gate[28] based on a single qubit. This gate has been extensively studied in the literature.[5,7,13–15,22] Our presentation here is only intended to set up the notation and illustrate methods useful in more complicated situations addressed in Sections 4, 6, 7, 8. We label by $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ the two basis states. The NOT gate corresponds to those interactions which, over the time interval Δt, accomplish the following:

$$\begin{pmatrix}1\\0\end{pmatrix} \Longrightarrow e^{i\alpha}\begin{pmatrix}0\\1\end{pmatrix}, \tag{1}$$

$$\begin{pmatrix}0\\1\end{pmatrix} \Longrightarrow e^{i\beta}\begin{pmatrix}1\\0\end{pmatrix}. \tag{2}$$

Here α and β are arbitrary. The unitary matrix U that corresponds to this evolution is

$$U = \begin{pmatrix}0 & e^{i\beta}\\ e^{i\alpha} & 0\end{pmatrix}, \tag{3}$$

with the eigenvalues

$$u_1 = e^{i(\alpha+\beta)/2} \qquad \text{and} \qquad u_2 = -e^{i(\alpha+\beta)/2}, \tag{4}$$

while the normalized eigenvectors yield the transformation matrix T which can be used to diagonalize U:

$$T = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{i\beta/2} & e^{i\beta/2}\\ e^{i\alpha/2} & -e^{i\alpha/2}\end{pmatrix}. \tag{5}$$

We have

$$T^{\dagger}UT = \begin{pmatrix}u_1 & 0\\ 0 & u_2\end{pmatrix}. \tag{6}$$

Here the dagger superscript denotes Hermitian conjugation.

We next use the relation

$$U = e^{-iH\Delta t/\hbar} \tag{7}$$

for a time-independent Hamiltonian. In the diagonal representation, it yields the energy levels:

$$E_1 = -\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{2\pi\hbar}{\Delta t}N_1, \qquad E_2 = -\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2+\frac{1}{2}\right), \tag{8}$$

where N_1 and N_2 are arbitrary integers. The Hamiltonian is then obtained from the relation

$$H = T\begin{pmatrix}E_1 & 0\\ 0 & E_2\end{pmatrix}T^{\dagger} \tag{9}$$

as a certain 2×2 matrix. The latter is conveniently represented is terms of the unit matrix $\mathcal{I}$ and the conventional Pauli matrices σ_x, σ_y, σ_z:

$$H = \left[-\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{\pi\hbar}{\Delta t}\left(N_1+N_2+\frac{1}{2}\right)\right]\mathcal{I} + \frac{\pi\hbar}{\Delta t}\left(N_1-N_2-\frac{1}{2}\right)\left[\left(\cos\frac{\alpha-\beta}{2}\right)\sigma_x + \left(\sin\frac{\alpha-\beta}{2}\right)\sigma_y\right]. \quad (10)$$

To effect the gate operation, the interaction must be switched on for the time interval Δt. The constant part of the Hamiltonian only affects the average phase $\frac{\alpha+\beta}{2}$ of the transformation (1)-(2). Thus this term can be disregarded.

The nontrivial part of (10) depends on the integer $N = N_1 - N_2$ which is arbitrary, and on one arbitrary variable

$$\gamma = \frac{\alpha-\beta}{2}. \quad (11)$$

Thus we can use the Hamiltonian

$$H = \frac{\pi\hbar}{\Delta t}\left(N-\frac{1}{2}\right)\left[(\cos\gamma)\,\sigma_x + (\sin\gamma)\,\sigma_y\right]. \quad (12)$$

For a spin-$\frac{1}{2}$ two-state system such an interaction can be obtained by applying a magnetic field oriented in the xy-plane at an angle γ with the x-axis. The strength of the field is inversely proportional to the desired time interval Δt, and various allowed field values are determined by the choice of N.

We note that during application of the external field the *up* and *down* quantum states in (1)-(2) are not the eigenstates of the Hamiltonian. If the time interval Δt is not short enough, the energy-level splitting $|E_1 - E_2| \propto |N - \frac{1}{2}|$ can result in spontaneous emission which is one of the sources of errors in computer operation. Generally, when implemented in condensed matter, the two states of the qubit may be part of a spectrum of many energy levels. In order to minimize the number of spontaneous transition modes, the best choice of the interaction strength would correspond to minimizing $|E_1 - E_2|$, i.e., to $|N - \frac{1}{2}| = \frac{1}{2}$.

4. THE SPATIALLY EXTENDED TWO-SPIN NOT GATE

In this section we consider a more complicated situation. Two two-state systems, input (I) and output (O), are involved. We will use the following self-explanatory notation for the state vector:

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = a_1|\uparrow\uparrow\rangle + a_2|\uparrow\downarrow\rangle + a_3|\downarrow\uparrow\rangle + a_4|\downarrow\downarrow\rangle$$

$$= a_1\begin{pmatrix}1\\0\end{pmatrix}_I \otimes \begin{pmatrix}1\\0\end{pmatrix}_O + a_2\begin{pmatrix}1\\0\end{pmatrix}_I \otimes \begin{pmatrix}0\\1\end{pmatrix}_O + a_3\begin{pmatrix}0\\1\end{pmatrix}_I \otimes \begin{pmatrix}1\\0\end{pmatrix}_O + a_4\begin{pmatrix}0\\1\end{pmatrix}_I \otimes \begin{pmatrix}0\\1\end{pmatrix}_O. \quad (13)$$

In what follows we will omit the direct-product symbols $\otimes$ when multiplying expressions with subscripts I and O.

We seek transformations such that irrespective of the initial state of O, and provided I is initially in the up or down state, the final state has O in the down or up state, respectively (while the final state of I is not restricted). Thus, we place the logical NOT of I in O provided the initial state of I was one of the basis states corresponding to the classical bit values 1 and 0. The desired transformation maps any state with $a_3 = a_4 = 0$ into a state with components 1 and 3 equal zero, i.e., input up yields output down. Similarly, any state with $a_1 = a_2 = 0$ should evolve into a state with components 2 and 4 equal zero, corresponding to input down giving output up. The general evolution operator must therefore be of the form

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} \\ U_{21} & U_{22} & 0 & 0 \\ 0 & 0 & U_{33} & U_{34} \\ U_{41} & U_{42} & 0 & 0 \end{pmatrix}, \tag{14}$$

which depends on 16 real parameters. However, one can show that the requirement of unitarity, $U^\dagger U = 1$, imposes 8 conditions so that the number of real parameters is reduced to 8. The following parametrization covers all such unitary matrices:

$$U = \begin{pmatrix} 0 & 0 & e^{i\chi}\sin\Omega & e^{i\beta}\cos\Omega \\ -e^{i(\alpha+\rho-\eta)}\sin\Upsilon & e^{i\rho}\cos\Upsilon & 0 & 0 \\ 0 & 0 & e^{i\delta}\cos\Omega & -e^{i(\beta+\delta-\chi)}\sin\Omega \\ e^{i\alpha}\cos\Upsilon & e^{i\eta}\sin\Upsilon & 0 & 0 \end{pmatrix}. \tag{15}$$

Here all the variables are unrestricted; we could limit Ω and Υ to the range $\left[0, \frac{\pi}{2}\right]$ without loss of generality.

In order to make the calculation analytically tractable, we will restrict the number of free parameters to four by considering the matrix

$$U = \begin{pmatrix} 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \end{pmatrix}. \tag{16}$$

This form has been favored for a possible analytical calculation for the following reasons. Firstly, the structure of a single phase-factor in each column is similar to that of the two-dimensional (single-spin) matrix encountered earlier. Secondly, the form (16) contains Hermitian-U cases ($\beta = -\alpha$, $\rho = 0$ or π, $\delta = 0$ or π). Therefore, the eigenvalues, which are generally on the unit circle for any unitary matrix, may be positioned symmetrically with respect to the real axis, as functions of the parameters. Indeed, the eigenvalues of U turn out to be quite simple:

$$u_1 = e^{i(\alpha+\beta)/2}, \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad u_3 = e^{i\rho}, \quad u_4 = e^{i\delta}. \tag{17}$$

The (unitary) diagonalizing matrix T is

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ e^{i\alpha/2} & -e^{i\alpha/2} & 0 & 0 \end{pmatrix}. \tag{18}$$

The next step is to identify the energy levels. We chose the notation such that the energies $E_{1,2}$ are identical to (8). The other two energies are given by

$$E_3 = -\frac{\hbar}{\Delta t}\rho + \frac{2\pi\hbar}{\Delta t}N_3, \quad E_4 = -\frac{\hbar}{\Delta t}\delta + \frac{2\pi\hbar}{\Delta t}N_4. \tag{19}$$

The Hamiltonian is then obtained as in the single-spin NOT case. It is convenient to avoid cumbersome expressions by expressing it in terms of the energies; the latter will be replaced by explicit expressions (8), (19) when needed. The resulting 4×4 matrix has been expressed in terms of the direct products involving the unit matrices and the Pauli matrices of the input and output two-state systems. We only report the result:

$$H = \frac{1}{4}(2E_1 + 2E_2 + E_3 + E_4) + \frac{1}{4}(E_3 - E_4)(\sigma_{zI} - \sigma_{zO}) + \frac{1}{4}(2E_1 + 2E_2 - E_3 - E_4)\sigma_{zI}\sigma_{zO}$$

$$+\frac{1}{4}(E_1-E_2)\left(\cos\frac{\alpha-\beta}{2}\right)(\sigma_{xI}\sigma_{xO}-\sigma_{yI}\sigma_{yO})+\frac{1}{4}(E_1-E_2)\left(\sin\frac{\alpha-\beta}{2}\right)(\sigma_{xI}\sigma_{yO}+\sigma_{yI}\sigma_{xO})\,. \quad (20)$$

The constant part of the Hamiltonian can be changed independently of the other coupling constants and it can be discarded. We can also generally vary the integers $N_{1,2,3,4}$ and the variables α, β, ρ, δ. The constant part is in fact proportional to $\mathcal{I}_I \otimes \mathcal{I}_O$. We avoid this notation and present the terms in the Hamiltonian in a more physically transparent form.

The Hamiltonian in (20) has also terms linear in the Pauli matrices (in the spin components for spin systems). These correspond to interactions with externally applied fields which in fact must be of opposite direction for the I and O spins. As explained in the introduction, we try to avoid such interactions: hopefully, external fields will only be used for clocking of the computation, i.e., for controlling the internal interactions via some intermediary part of the system connecting the I and O two-state systems. Thus, we will assume that $E_3 = E_4$ so that there are no terms linear is the spin components.

Among the remaining interaction terms, the term involving the z-components in the product form $\sigma_{zI}\sigma_{zO}$ ($\equiv \sigma_{zI} \otimes \sigma_{zO}$), has an arbitrary coefficient to be denoted $-\mathcal{E}$. The terms of order two in the x and y components have free parameters similar to those in (11)-(12). The final expression is

$$H = -\mathcal{E}\sigma_{zI}\sigma_{zO} + \frac{\pi\hbar}{2\Delta t}\left(N-\frac{1}{2}\right)\Big[(\cos\gamma)(\sigma_{xI}\sigma_{xO}-\sigma_{yI}\sigma_{yO})+(\sin\gamma)(\sigma_{xI}\sigma_{yO}+\sigma_{yI}\sigma_{xO})\Big]\,. \quad (21)$$

Here $N = N_1 - N_2$ must be an integer. In order to minimize the spread of the energies E_1 and E_2 we could choose $|N-\frac{1}{2}| = \frac{1}{2}$. Recall that we already have $E_3 = E_4$. Thus the energy levels of the Hamiltonian in (21) are

$$E_1 = -\mathcal{E} + \frac{\pi\hbar}{\Delta t}\left(N-\frac{1}{2}\right)\,, \quad E_2 = -\mathcal{E} - \frac{\pi\hbar}{\Delta t}\left(N-\frac{1}{2}\right)\,, \quad E_{3,4} = \mathcal{E}\,. \quad (22)$$

Thus degeneracy of three levels (but not all four) can be achieved by varying the parameters.

The form of the interactions (21) is quite unusual as compared to the traditional spin-spin interactions in condensed matter models. The latter usually are based on the uniaxial (Ising) interaction proportional to $\sigma_z\sigma_z$, or the planar XY-model interaction proportional to $\sigma_x\sigma_x + \sigma_y\sigma_y$, or the isotropic (scalar-product) Heisenberg interaction. The spin components here are those of two different spins (not marked). The interaction (21) involves an unusually high degree of anisotropy in the system. The x and y components are coupled in a tensor form which presumably will have to be realized in a medium with well-defined directionality, possibly, a crystal.

5. COMMENT ON TIME-DEPENDENCE OF INTERACTIONS

The Hamiltonians considered thus far were all constant for the duration of the gate operation. We note that the external control of the interaction need not be limited to the time-dependence which is an abrupt on/off switching. Indeed, we can modify the time dependence according to

$$H(t) = f(t)H\,, \quad (23)$$

where we use the same symbol H for both the original time-independent interaction Hamiltonian such as (21) and the new, time-dependent one, $H(t)$. The latter involves the protocol function $f(t)$. The shape of this function, nonzero during the operation of the gate from time t to time $t+\Delta t$, can be smooth.

For Hamiltonians involving externally applied fields, such as (12), it may be important to have a constant plus an oscillatory components (corresponding to constant and electromagnetic-wave magnetic fields, for instance). However, the protocol function must satisfy

$$\int_t^{t+\Delta t} f(t')\,dt' = \Delta t\,, \quad (24)$$

and therefore it cannot be purely oscillatory; it must have a constant or other contribution to integrate to a nonzero value in accordance with (24).

The possibility of the modification (23) follows from the fact that the general relation

$$U = \left[e^{-i \int_t^{t+\Delta t} H(t')\, dt'/\hbar} \right]_{\text{time-ordered}} \tag{25}$$

does not actually require time ordering as long as the Hamiltonian commutes with itself at different times. This condition is satisfied by (23). Furthermore, if the Hamiltonian can be written as a sum of commuting terms then each term can be multiplied by its own protocol function. Interestingly, the Hamiltonian of the paramagnetic-resonance NOT gate[14] is not of this form. It contains a constant part and an oscillatory part but they do not commute. Note that the term proportional to $\mathcal{E}$ in (21) commutes with the rest of that Hamiltonian. The terms proportional to $\cos\gamma$ and $\sin\gamma$ do not commute with each other. Rather, they anticommute, in (21), as such terms do in (12).

6. THE THREE-SPIN XOR GATE

Thus far we learned that extending the number of spins (qubits, two-state systems) involved in the NOT gate from one to two produced an interaction Hamiltonian family (21) with structure that is quite new and unfortunately not symmetric in terms of what we are used to in solid-state magnetic interactions. We will now consider a *three-spin system*: a quantum-XOR gate (which can also be realized[10,30,43] with two spins). This choice is dictated by the fact that we can obtain analytical results and address a new issue that was not there for one- or two-spin systems: whether this quantum gate function can be accomplished with two-spin interactions.

We note that if a quantum logic operation is allowed to be decomposed into a sequence of unlimited number of universal one- and two-spin gates then one can always reduce it to two-spin interactions.[5,7,15,44] Here, however, we are interested in one-shot gates for which the external control involves the overall system Hamiltonian, over a single time interval Δt. The possibility of using solely two-spin interactions will actually depend on the logical function and for more complicated systems it has to be explored by numerical studies. We note also that the issue of having the interactions short-range (e.g., nearest-neighbor) does not really arise for few-spin systems although it will be an important design criterion as the number of spins (qubits) involved increases. Short-range two-particle interactions are much better studied and accessible to experimental probe than multi-particle interactions.

We denote by A, B, C the three two-state systems, i.e., three spins (qubits). The transformation must be specified for those initial states of the input spins A and B, at time t, that are one of the basis states $|AB\rangle = |11\rangle$, $|10\rangle$, $|01\rangle$, or $|00\rangle$, where 1 and 0 denote the eigenstates of the z-components of the spin operators. Here 1 refers to the up state and 0 refers to the down state; we use this notation for consistency with the classical bit notion. The initial state of C is not specified. We would like to have a quantum evolution that mimics the XOR function:

A	B	output
1	1	0
1	0	1
0	1	1
0	0	0

(26)

Here the output is at time $t + \Delta t$. One way to accomplish this is to produce the output in A or B, i.e., work with a two-spin system where the input and output are the same. The Hamiltonian for such a system is not unique. Explicit examples can be found[10,30] where XOR was obtained as a sub-result of the controlled-NOT gate operation. In the case of two spins involved, the interactions can be single- and two-spin only.

Here we require that the XOR result be put in C at time $t + \Delta t$. The final states of A and B, as well as the phase of C are arbitrary. In fact, there are many different unitary transformations, U, that correspond to the desired evolution in the eight-state space with the basis $|ABC\rangle = |111\rangle$, $|110\rangle$, $|101\rangle$, $|100\rangle$, $|011\rangle$, $|010\rangle$, $|001\rangle$, $|000\rangle$. The choice of the transformation determines what happens when the initial state is a superposition of the reference states, what are the phases in the output, etc.

Let us consider first the following Hamiltonian[31,32]

$$H = \frac{\pi\hbar}{4\Delta t}\left(\sqrt{2}\sigma_{zA}\sigma_{yB} + \sqrt{2}\sigma_{zB}\sigma_{yC} - \sigma_{yB}\sigma_{xC}\right). \tag{27}$$

It is written here in terms of the spin components; the subscripts A, B, C denote the spins. In the eight-state basis specified earlier, its matrix can be obtained by direct product of the Pauli matrices and unit 2×2 matrices $\mathcal{I}$. For instance, the first interaction term is proportional to $\sigma_{zA} \otimes \sigma_{yB} \otimes \mathcal{I}_C$, This Hamiltonian involves only two-spin-component interactions. In fact, in this particular example A and C only interact with B.

One can show that the Hamiltonian (27) corresponds to the XOR result in C at $t + \Delta t$ provided A and B were in one of the allowed superpositions of the appropriate binary states at t (we refer to superposition here because C is arbitrary at t). There are two ways to verify this.[31,32] Firstly, one can diagonalize H and then calculate the evolution matrix U in the diagonal representation by using the general relation (7), valid for Hamiltonians which are constant during the time interval Δt, and then reverse the diagonalizing transformation.

The second, more general approach presented here is to design a whole family of two-spin-interaction Hamiltonians of which the form (27) is but a special case, by analyzing generally a family of 8×8 unitary matrices corresponding to the three-spin XOR gate. This program is carried out in Sections 7, 8.

7. THE STRUCTURE OF THE XOR UNITARY MATRIX AND HAMILTONIAN

We require any linear combination of the states $|\underline{1}11\rangle$ and $|\underline{1}10\rangle$ to evolve into a linear combination of $|1\underline{1}0\rangle$, $|1\underline{0}0\rangle$, $|0\underline{1}0\rangle$, and $|0\underline{0}0\rangle$; compare the underlined quantum numbers with the first entry in (26), with similar rules for the other three entries in (26). In the matrix notation, and in the standard basis $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, the most general XOR evolution operator corresponding to the Boolean function (26), with the output in C, is, therefore,

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} & U_{15} & U_{16} & 0 & 0 \\ U_{21} & U_{22} & 0 & 0 & 0 & 0 & U_{27} & U_{28} \\ 0 & 0 & U_{33} & U_{34} & U_{35} & U_{36} & 0 & 0 \\ U_{41} & U_{42} & 0 & 0 & 0 & 0 & U_{47} & U_{48} \\ 0 & 0 & U_{53} & U_{54} & U_{55} & U_{56} & 0 & 0 \\ U_{61} & U_{62} & 0 & 0 & 0 & 0 & U_{67} & U_{68} \\ 0 & 0 & U_{73} & U_{74} & U_{75} & U_{76} & 0 & 0 \\ U_{81} & U_{82} & 0 & 0 & 0 & 0 & U_{87} & U_{88} \end{pmatrix}. \tag{28}$$

The condition of unitarity, $UU^\dagger = 1$, reduces the number of independent parameters but they are still too numerous for the problem to be manageable analytically; we are going to consider a subset of operators of this form.

From our earlier discussion we know that one way to reduce the number of parameters and ensure unitarity is to keep a single phase factor in each column and row of the matrix. Some amount of lucky guessing is involved in finding an analytically tractable parametrization. Thus, we choose a form which is diagonal in the states of the A-spin,

$$U = \begin{pmatrix} V_{4\times4} & 0_{4\times4} \\ 0_{4\times4} & W_{4\times4} \end{pmatrix}. \tag{29}$$

Note that the input spins A and B are not treated symmetrically. Here $0_{4\times4}$ denotes the 4×4 matrix of zeros. The 4×4 matrices V and W are parametrized as follows:

$$V = \begin{pmatrix} 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\gamma} & 0 & 0 \end{pmatrix}, \tag{30}$$

$$W = \begin{pmatrix} 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & 0 & e^{i\omega} \\ e^{i\xi} & 0 & 0 & 0 \\ 0 & 0 & e^{i\eta} & 0 \end{pmatrix} . \tag{31}$$

This choice of an 8-parameter unitary matrix U, see (29), was made because it has the structure

$$2U = (1+\sigma_{zA})\,V + (1-\sigma_{zA})\,W = V + W + \sigma_{zA}(V-W)\,, \tag{32}$$

where V and W are operators in the space of B and C. Since U was chosen diagonal in the space of A, the Hamiltonian, H, will have a similar structure,

$$2H = P + Q + \sigma_{zA}(P-Q)\,, \tag{33}$$

with the appropriate Hamiltonians P and Q in the $(B \otimes C)$-space. In order to avoid three-spin interactions, $P-Q$ must be linear in the Pauli matrices. We also try to avoid single-spin (external-field) interactions. Thus, $P+Q$ must contain only terms of the second order in the spin components while $P-Q$ must contain only terms of the first order in the spin components. This suggests avoiding putting phase factors on the diagonal, which would lead to matrices similar to those encountered in extended-NOT-gate calculations that are known to be of a structure undesirable here: they contain a mixture of first-order and second-order terms. The off-diagonal choices remaining are considerably limited: the forms (30)-(31) are nearly unique.

In summary, while the arguments are admittedly vague and they do involve a certain level of guess, trial and error, the presented parametrization offers a good chance that with further restrictions on the parameters a two-spin interaction Hamiltonian can be obtained. As will be seen shortly, five conditions are imposed so that the resulting Hamiltonian depends on three (real) parameters.

Let us define

$$\mu = \frac{\alpha+\beta+\gamma+\delta}{4}\,, \quad \nu = \frac{\rho+\omega+\xi+\eta}{4}\,, \tag{34}$$

and introduce the reduced operators p and q,

$$P = -\frac{\hbar}{\Delta t}p \quad \text{and} \quad Q = -\frac{\hbar}{\Delta t}q\,, \tag{35}$$

Then (7) yields

$$V = \exp(ip) \quad \text{and} \quad W = \exp(iq)\,. \tag{36}$$

Next, we diagonalize V and W: we calculate their eigenvalues and also the matrices of their normalized eigenvectors, in order to transform to the diagonal representations.

Specifically, the eigenvalues of V are $e^{i\mu}$, $ie^{i\mu}$, $-e^{i\mu}$, $-ie^{i\mu}$. The appropriate eigenvalues of p then follow form (36) as μ, $\mu+\frac{1}{2}\pi$, $\mu+\pi$, $\mu+\frac{3}{2}\pi$. Arbitrary multiples of 2π can be added to these choices. However, there are certain nonrigorous arguments for generally keeping the spread of eigenvalues of the Hamiltonian as small as possible. Thus, we choose the simplest expressions. The eigenvalues of q are determined identically, with μ replaced by ν throughout.

The next step is to apply the inverse of the diagonalizing transformations for V and W to the diagonal 4×4 matrices for, respectively, p and q. The latter contain the eigenvalues of p and q as the diagonal elements. The results are the matrix forms of the operators p and q in the original representation:

$$\frac{4}{\pi}p = \begin{pmatrix} \frac{4}{\pi}\mu+3 & -(1+i)e^{i(\mu-\alpha)} & -(1-i)e^{i(\delta-\mu)} & -e^{i(2\mu-\alpha-\gamma)} \\ -(1-i)e^{i(\alpha-\mu)} & \frac{4}{\pi}\mu+3 & -e^{i(2\mu-\beta-\gamma)} & -(1+i)e^{i(\mu-\gamma)} \\ -(1+i)e^{i(\mu-\delta)} & -e^{i(\beta+\gamma-2\mu)} & \frac{4}{\pi}\mu+3 & -(1-i)e^{i(\beta-\mu)} \\ -e^{i(\alpha+\gamma-2\mu)} & -(1-i)e^{i(\gamma-\mu)} & -(1+i)e^{i(\mu-\beta)} & \frac{4}{\pi}\mu+3 \end{pmatrix}, \tag{37}$$

$$\frac{4}{\pi}q = \begin{pmatrix} \frac{4}{\pi}\nu+3 & -(1-i)e^{i(\rho-\nu)} & -(1+i)e^{i(\nu-\xi)} & -e^{i(\rho+\omega-2\nu)} \\ -(1+i)e^{i(\nu-\rho)} & \frac{4}{\pi}\nu+3 & -e^{i(\omega+\eta-2\nu)} & -(1-i)e^{i(\omega-\nu)} \\ -(1-i)e^{i(\xi-\nu)} & -e^{i(2\nu-\omega-\eta)} & \frac{4}{\pi}\nu+3 & -(1+i)e^{i(\nu-\eta)} \\ -e^{i(2\nu-\rho-\omega)} & -(1+i)e^{i(\nu-\omega)} & -(1-i)e^{i(\eta-\nu)} & \frac{4}{\pi}\nu+3 \end{pmatrix}. \tag{38}$$

8. THE TWO-SPIN-INTERACTION XOR HAMILTONIAN

Thus far we decreased the number of independent parameters in the general unitary transformation and chose it to be diagonal in the A-space. We now refine our design of the Hamiltonian to favor interaction of the second order in the Pauli matrices. First, we note that both P and Q are constant-diagonal matrices. Therefore, in terms of the Pauli matrices both their sum and difference in (33) will involve constant terms. These are undesirable because in $\sigma_{zA}(P-Q)$ they lead to terms of order one (instead of the desired two), in H, while in $P+Q$ they lead to an additive constant in H which only affects the overall phase of the unitary transformation and is of no interest otherwise. Therefore, we put

$$\mu = \nu = -\frac{3}{4}\pi, \tag{39}$$

in order to nullify these diagonal elements in both P and Q.

Let us now focus our attention on $P-Q$ which, by (39), is now a matrix with zero diagonal. We must impose conditions on the parameters to make $P-Q$ of order exactly one in the Pauli matrices. We note, however, that due to zero-diagonal, it cannot contain σ_z terms. The general form liner in σ_x, σ_y is

$$P-Q = \mathcal{I}_B \otimes \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}_C + \begin{pmatrix} 0 & Y \\ Y^* & 0 \end{pmatrix}_B \otimes \mathcal{I}_C = \begin{pmatrix} 0 & X & Y & 0 \\ X^* & 0 & 0 & Y \\ Y^* & 0 & 0 & X \\ 0 & Y^* & X^* & 0 \end{pmatrix}, \tag{40}$$

where the stars denote complex conjugation, X and Y are arbitrary (complex) numbers, and $\mathcal{I}$ stands for the unit matrix as before. Thus we require that $P-Q$ be of the form suggested by (40). This imposes several conditions: two above-diagonal elements of the difference must be equal to zero while the remaining four elements must be equal pairwise. One can show that these conditions are satisfied provided α, β, γ are kept as three independent (real) parameters while the remaining angles are given by

$$\delta = -3\pi - \alpha - \beta - \gamma, \tag{41}$$

$$\rho = -\pi + \beta, \tag{42}$$

$$\omega = -2\pi - \alpha - \beta - \gamma, \tag{43}$$

$$\xi = -\pi + \gamma, \tag{44}$$

$$\eta = \pi + \alpha. \tag{45}$$

Note that (39) is built into (41)-(45). Given this choice, it turns out that $P+Q$ contains only two-spin interactions. We have no simple explanation of this property (of the absence of first-order terms in $P+Q$). It is probably related to the fact that the structure pattern of the original matrices V and W is quite similar even though the precise positioning of nonzero elements is different. We find

$$P+Q=-\frac{\sqrt{2}\pi\hbar i}{4\Delta t}\begin{pmatrix} 0 & e^{-i\alpha}+e^{i\beta} & e^{-i(\alpha+\beta+\gamma)}-e^{-i\gamma} & -\sqrt{2}e^{-i(\alpha+\gamma)} \\ -e^{i\alpha}-e^{-i\beta} & 0 & -\sqrt{2}e^{-i(\beta+\gamma)} & e^{-i\gamma}-e^{-i(\alpha+\beta+\gamma)} \\ e^{i\gamma}-e^{i(\alpha+\beta+\gamma)} & \sqrt{2}e^{i(\beta+\gamma)} & 0 & -e^{-i\alpha}-e^{i\beta} \\ \sqrt{2}e^{i(\alpha+\gamma)} & e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & e^{i\alpha}+e^{-i\beta} & 0 \end{pmatrix}, \quad (46)$$

$$P-Q=-\frac{\sqrt{2}\pi\hbar i}{4\Delta t}\begin{pmatrix} 0 & e^{-i\alpha}-e^{i\beta} & e^{-i(\alpha+\beta+\gamma)}+e^{-i\gamma} & 0 \\ -e^{i\alpha}+e^{-i\beta} & 0 & 0 & e^{-i(\alpha+\beta+\gamma)}+e^{-i\gamma} \\ -e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & 0 & 0 & e^{-i\alpha}-e^{i\beta} \\ 0 & -e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & -e^{i\alpha}+e^{-i\beta} & 0 \end{pmatrix}, \quad (47)$$

Finally, we expand these matrices in terms of products of the Pauli matrices and collect terms according to (33) to get

$$\begin{aligned} H=-\frac{\pi h}{8\Delta t}\Big\{ & \sqrt{2}\,(\sin\alpha+\sin\beta)\,\sigma_{zA}\sigma_{xC}-\sqrt{2}\,(\cos\alpha-\cos\beta)\,\sigma_{zA}\sigma_{yC}+\sqrt{2}\big[\sin\gamma+\sin(\alpha+\beta+\gamma)\big]\sigma_{zA}\sigma_{xB} \\ & -\sqrt{2}\big[\cos\gamma+\cos(\alpha+\beta+\gamma)\big]\sigma_{zA}\sigma_{yB}+\sqrt{2}\,(\sin\alpha-\sin\beta)\,\sigma_{zB}\sigma_{xC}-\sqrt{2}\,(\cos\alpha+\cos\beta)\,\sigma_{zB}\sigma_{yC} \\ & -\sqrt{2}\big[\sin\gamma-\sin(\alpha+\beta+\gamma)\big]\sigma_{xB}\sigma_{zC}+\sqrt{2}\big[\cos\gamma-\cos(\alpha+\beta+\gamma)\big]\sigma_{yB}\sigma_{zC}-\big[\sin(\alpha+\gamma)+\sin(\beta+\gamma)\big]\sigma_{xB}\sigma_{xC} \\ & +\big[\cos(\alpha+\gamma)-\cos(\beta+\gamma)\big]\sigma_{xB}\sigma_{yC}+\big[\cos(\alpha+\gamma)+\cos(\beta+\gamma)\big]\sigma_{yB}\sigma_{xC}+\big[\sin(\alpha+\gamma)-\sin(\beta+\gamma)\big]\sigma_{yB}\sigma_{yC}\Big\}. \end{aligned} \quad (48)$$

Note that (27) corresponds to the parameter choice $\alpha=\beta=\gamma=0$. The Hamiltonian (48) describes the three-spin XOR. For arbitrary values of α,β,γ, the interactions involved are all two-spin as desired. The result, however, is not symmetric in any obvious way. It seems to correspond to complicated tensor interactions involving expressions of order two in the components of the three spins involved. No rotational or other symmetry in the three-component spin space, or planar symmetry, or uniaxial coupling, are apparent. All these would correspond to the familiar Heisenberg, XY, and Ising couplings in condensed matter physics.

Thus, in order to realize interaction (48) in materials, a rather anisotropic medium with highly nonsymmetric tensorial magnetic interactions will be required. In this respect our analytical attempt to design a multi-spin quantum gate cannot be considered really successful. While we learned several general principles, the unappealing form of the Hamiltonians (21) and (48) suggests that different roots to the derivation of Hamiltonians should be also explored. One could start with the more conventional magnetic interactions, isotropic (Heisenberg), planar (XY), uniaxial (Ising), and explore general-parameter Hamiltonians, adjusting the coupling parameters numerically in search of those values for which useful Boolean gate operations are carried out. Another approach would be to use, in input and output, quantum states more general than the logic products of the qubit-basis-states which are presently favored because of the correspondence with classical computers. Then the design of Hamiltonians may be easier but there is a trade-off. These devices will have to be incorporated into larger computers or interact with classical (i.e., dissipative) computer components. Radically new programming ideas will be needed to use transformations that connect *superpositions* of qubit states to carry out computations.

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4.0 RESEARCH ARTICLE

ADIABATIC DECOHERENCE

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KEY WORDS: Quantum decoherence, heat bath, effects of environment, dissipation

ABSTRACT

We study a general quantum system interacting with environment modeled by the bosonic heat bath of Caldeira and Leggett type. General interaction Hamiltonians are considered that commute with the system's Hamiltonian so that there is no energy exchange between the system and bath. We argue that this model provides an appropriate description of adiabatic quantum decoherence, i.e., loss of entanglement on time scales short compared to those of thermal relaxation processes associated with energy exchange with the bath. The interaction Hamiltonian is then proportional to a conserved "pointer observable." Calculation of the elements of the reduced density matrix of the system is carried out exactly, and time-dependence of decoherence is identified, similar to recent results for related models. Our key finding is that the decoherence process is controlled by spectral properties of the interaction rather than system's Hamiltonian.

1. Introduction

Quantum decoherence, dissipation, and thermalization due to interactions with environment have long been important fundamental issues theoretically and experimentally.[1-11] Decoherence and related topics have attracted much interest recently due to rapid development of new fields such as quantum computing and quantum information theory.[12-18] Decoherence due to external interactions is a major obstacle in the way of implementation of devices such as quantum computers. Thus in addition to studies of the physics of decoherence processes there emerged a new field of quantum error correction[19-25] aiming at effective stabilization of quantum states against decoherence essentially by involving many additional quantum systems and utilizing redundancy. The present work contributes to the former topic: the physics of decoherence.

Decoherence is a result of the coupling of the quantum system under consideration to the environment which, generally, is the rest of the universe. In various experimentally relevant situations the interaction of the quantum system with environment is dominated by the system's microscopic surroundings. For example, the dominant source of such interaction for an atom in an electromagnetic cavity is the electromagnetic field itself coupled to the dipole moment of the atom.[26] In case of Josephson

junction in a magnetic flux[27] or defect propagation in solids, the interaction can be dominated by acoustic phonons or delocalized electrons.[28] Magnetic macromolecules interact with the surrounding spin environment such as nuclear spins.[18] Numerous other specific examples could be cited.

In this work we aim at a general phenomenological description that models the physically important effects of external interactions as far as adiabatic decoherence, to be defined later, is concerned. We note that generally thermalization and decoherence are associated with the interaction of the quantum system, described in isolation by the Hamiltonian H_S, with another, large system which we will term the "bath" and which internally has the Hamiltonian H_B. The actual interaction will be represented by the Hamiltonian H_I so that the total Hamiltonian of the system, H, is

$$H = H_S + H_B + H_I \,. \tag{1.1}$$

It is important to realize that typically the bath is a large, macroscopic system. Truly irreversible interactions of a quantum system with its environment, such as thermal equilibration or decoherence associated with measurement processes, can only be obtained in the Hamiltonian description (1.1) when it is supplemented by taking the limit of the number of

particles or degrees or freedom of the bath going to infinity.

Interactions of a quantum system with macroscopic systems can lead to different outcomes. For instance, interaction with a true "heat bath" leads to thermalization: the reduced density matrix of the system approaches $\exp(-\beta H_S)$ for large times. Here

$$\beta = 1/(kT) \tag{1.2}$$

as usual, and by "reduced" we mean the density matrix traced over the states of the bath. On the other hand in decoherence we expect the reduced density matrix to approach a diagonal form in the "preferred basis" somehow selected by the "pointer observable" Hermitian operator[1-6,29,30] which is thereby "measured" by the macroscopic system (bath).

It is important to realize that study of decoherence in the present context does not fully resolve the problem of understanding quantum measurement and other fundamental issues at the borderline of quantum and classical behaviors, such as, for instance, the absence of macroscopic manifestations of Schrödinger-cat type quantum superposition of states. The more optimistic recent literature[4-6] considers description of entanglement and decoherence the key to such understanding. However, these fundamental problems have remained open thus far.

The most explored and probably most tractable approach to modeling the environmental interactions has involved representing their effects by coupling the original quantum system to a set of noninteracting harmonic oscillators (bosonic heat bath).[1,2,8–11,14,31–33] Fermionic heat bath can be also considered, e.g., Ref. 34. We will use the term "heat bath" for such systems even when they are used for other then thermalization studies because they have the temperature parameter defined via initial conditions, as described later.

Rigorous formulation of the bosonic heat bath approach was initiated by Ford, Kac and Mazur[32] and more recently by Caldeira and Leggett.[11,29] It has been established, for harmonic quantum systems. that the influence of the heat bath described by the oscillators is effectively identical to the external uncorrelated random force acting on a quantum system under consideration. In order for the system to satisfy equation of motion with a linear dissipation term in the classical limit the coupling was chosen to be linear in coordinates while the coupling constants entered lumped in a spectral function which was assumed to be of a power-law form in the oscillator frequency, with the appropriate Debye cutoff. We will make this concept more explicit later.

This model of a heat bath was applied to studying effects of dissipation on the probability of quantum tunneling from a metastable

state.[8,29] It was found that coupling a quantum system to the heat bath actually decreases the quantum tunneling rate. The problem of a particle in a double well potential was also considered.[9,33] In this case the interaction with the bath leads to quantum coherence loss and complete localization at zero temperature. This study has lead to the spin-boson Hamiltonian[9,10] which found numerous other applications. The Hilbert space of the quantum systems studied was effectively restricted to the two-dimensional space corresponding to the two lowest energy levels.

Another possible application of the bosonic heat bath model concerns aspects of quantum measurement. It is believed that the bath is an intrinsic part of a measuring device. In other words, it continuously monitors the physical quantity whose operator is coupled to it.[4–6] It has been shown in the exactly solvable model of the quantum oscillator coupled to a heat bath[5] that the reduced density matrix of the quantum system decoheres, i.e., looses its off-diagonal elements representing the quantum correlations in the system, in the eigenbasis of the interaction Hamiltonian. It has also been argued that the time scale on which this "measurement" occurs is much less than the characteristic time for thermal relaxation of the system.

It is natural to assume that if such a "bath" description of the process of measurement of a Hermitian operator Λ_S exists, then the inter-

action Hamiltonian H_I in (1.1) will involve Λ_S as well as some bath-Hilbert-space operators. No general description of this process exists. Furthermore, when we are limited to specific models in order to obtain tractable, e.g., analytically solvable, examples, then there is no general way to separate decoherence and thermalization effects. We note that thermalization is naturally associated with exchange of energy between the quantum system and heat bath. Model system results and general expectations mentioned earlier suggest that at least in some cases decoherence involves its own time scales which are shorter than those of approach to thermal equilibrium.

In this work we propose to study adiabatic decoherence, i.e., a special case of no energy exchange between the system and bath. Thus we assume that H_S is conserved, i.e., $[H_S, H] = 0$. This assumption is a special case of "quantum nondemolition measurement" concept[2,30] exemplified by the Kerr effect, for instance. Since H_S and H_B is (1.1) operate in different Hilbert spaces, this is equivalent to requiring

$$[H_S, H_I] = 0\,. \tag{1.3}$$

Furthermore, we will assume that H_I is linear in Λ_S:

$$H_I = \Lambda_S P_B\,, \tag{1.4}$$

where P_B acts in the Hilbert space of the bath. Then we have

$$[\Lambda_S, H_S] = 0\,. \tag{1.5}$$

Thus, we consider cases in which the measured, "pointer" observable Λ_S is one of the conserved quantities of the quantum system when it is isolated. Interaction with the bath will then correspond to measurement of such an observable, which can be the energy itself. Specifically, the model of Ref. 14 corresponds to $\Lambda_S = H_S$ for the case of the spin-$\frac{1}{2}$ two-state system, motivated by quantum-computing applications; see also Refs. 2, 12-15. The models of Refs. 1 and 2 correspond to the choices of $\Lambda_S = H_S$ and $\Lambda_S = f(H_S)$, respectively, for a system coupled to a bosonic spin bath, where f is an arbitrary well-behaved function.

Here we derive exact results for adiabatic decoherence due to coupling to the bosonic heat bath, assuming general Λ_S that commutes with H_S. While technically this represents an extension of the results of Refs. 1 and 2, we demonstrate that the general case reveals certain new aspects of the decoherence process. Our new exact-solution method utilizes coherent states and may be of interest in other applications as well. In Section 2, we define the system. Specifically, we choose the bosonic heat bath form for H_B and P_B in (1.1) and (1.4), but we keep H_S and Λ_S general. However, we also analyze the mechanism leading to exact solvability of

general models of this type. Section 3 reports our derivation of the exact expression for the reduced density matrix of the system. Discussion of the results and definition of the continuum limit are given in Section 4.

2. Models of Adiabatic Decoherence

We will be mainly interested in the following Hamiltonian for the quantum system coupled to a bath of bosons (harmonic oscillators) labeled by the subscript k:

$$H = H_S + \sum_k \omega_k a_k^\dagger a_k + \Lambda_S \sum_k \left(g_k^* a_k + g a_k^\dagger \right) . \tag{2.1}$$

Here $a_k^\dagger$ and a_k are bosonic creation and annihilation operators, respectively, so that their commutation relation is $[a_k, a_k^\dagger] = 1$. The second term in (2.1) represents the free field or Hamiltonian of the heat bath H_B. The last term is the interaction Hamiltonian H_I. The coupling constants will be specified later; exact results obtained in Section 3 apply for general ω_k and g_k. Here and in the following we use the convention

$$\hbar = 1 \tag{2.2}$$

and we also assume that the energy levels of each oscillator are shifted by $\frac{1}{2}\omega_k$ so that the ground state of each oscillator has zero energy.

Since we assume that H_S and Λ_S commute, we can select a common set $|i\rangle$ of eigenstates:

$$H_S|i\rangle = E_i|i\rangle\,, \tag{2.3}$$

$$\Lambda_S|i\rangle = \lambda_i|i\rangle\,. \tag{2.4}$$

One of the simplifications here, due to the fact that H_S and Λ_S commute, is that these eigenstates automatically constitute the "preferred basis" mentioned earlier.

We will assume that initially the quantum system is in a pure or mixed state described by the density matrix $\rho(0)$, not entangled with the bath. For the bath, we assume that each oscillator is independently thermalized (possibly by prior contact with a "true" heat bath) at temperature T, with the density matrix θ_k. The total system-plus-bath density matrix will then be the product

$$\rho(0)\prod_k \theta_k\,. \tag{2.5}$$

Here

$$\theta_k = Z_k^{-1} e^{-\beta\omega_k a_k^\dagger a_k}\,, \tag{2.6}$$

$$Z_k \equiv (1 - e^{-\beta\omega_k})^{-1}\,, \tag{2.7}$$

where Z_k is the partition function for the oscillator k. The quantity β was defined in (1.2). Introduction of the temperature parameter via the initial state of the bath is common in the literature.[1,2,8–11,14–17,29,32,33] While it may seem artificial, we recall that the bath is supposed to be a large system presumably remaining thermalized on the time scales of interest. Specific results indicating that the bosonic heat bath can be viewed as a source of thermalizing noise have been mentioned earlier; see also Ref. 35.

Our objective is to study the reduced density matrix of the system at time $t \geq 0$; it has the following matrix elements in the preferred basis:

$$\rho_{mn}(t) = \mathrm{Tr}_B \left[\langle m|e^{-iHt} \left(\rho(0) \prod_k \theta_k \right) e^{iHt}|n\rangle \right] . \tag{2.8}$$

Here the outer trace is taken over the states of the heat bath, i.e., the bosonic modes. The inner matrix element is in the space of the quantum system. Note that for no coupling to the bath, i.e., for $g_k = 0$, the density matrix of the system is simply

$$[\rho_{mn}(t)]_{g_k=0} = \rho_{mn}(0)e^{i(E_n - E_m)t} . \tag{2.9}$$

For the interacting system, the heat-bath states must be summed over in the trace in (2.8). It is instructive to consider a more general case with the bath consisting of independent "modes" with the Hamiltonians M_k, so that

$$H_B = \sum_k M_k \,, \tag{2.10}$$

where for the bosonic bath we have $M_k = \omega_k a_k^\dagger a_k$. Similarly, for the interaction term we assume coupling to each mode independently,

$$H_I = \Lambda_S \sum_k J_k \,, \tag{2.11}$$

where for the bosonic bath we have $J_k = g_k^* a_k + g a_k^\dagger$. Relation (2.5) remains unchanged, with the definitions (2.6) and (2.7) replaced by

$$\theta_k = Z_k^{-1} e^{-\beta M_k} \,, \tag{2.12}$$

$$Z_k = \mathrm{Tr}_k \left[e^{-\beta M_k} \right] \,, \tag{2.13}$$

where the trace is over a single mode k.

Owing to the fact that H_S and Λ_S share common eigenfunctions,

the inner matrix element calculation in (2.8), in the system space, can be expressed in terms of the eigenvalues defined in (2.3)-(2.4). Specifically, we define the bath-space operators

$$h_i = E_i + \sum_k M_k + \lambda_i \sum_k J_k \,, \tag{2.14}$$

which follow from the form of the Hamiltonian. The calculation in (2.8) then reduces to

$$\rho_{mn}(t) = \mathrm{Tr}_B \left[\langle m| e^{-ih_m t} \left(\rho(0) \prod_k \theta_k \right) e^{ih_n t} |n\rangle \right] , \tag{2.15}$$

which yields the expression

$$\rho_{mn}(t) = \rho_{mn}(0) \mathrm{Tr}_B \left[e^{-ih_m t} \left(\prod_k \theta_k \right) e^{ih_n t} \right] . \tag{2.16}$$

We will now assume that the operators of different modes k commute. This is obvious for the bosonic or spin baths and must be checked explicitly if one uses the present formulation for a fermionic bath. Then we can factor the expression (2.16) as follows:

$$\rho_{mn}(t) = \rho_{mn}(0) e^{i(E_n - E_m)t} \prod_k \left\{ \mathrm{Tr}_k \left[e^{-i(M_k + \lambda_m J_k)t} \theta_k e^{i(M_k + \lambda_n J_k)t} \right] \right\} . \tag{2.17}$$

This expression, or variants derived in earlier works,[1,2,14] suggests that the problem is exactly solvable in some cases. Indeed, the inner trace in over a single mode of the bath. For a spin bath of spin-$\frac{1}{2}$ "modes" the calculation involves only (2×2)-matrix manipulations and is therefore straightforward.[2,14] However, in this case the only nontrivial choice of the "pointer observable" corresponds, in our notation, to $\Lambda_S = H_S$, with both operators usually chosen equal to the Pauli matrix σ_z. There is also hope for obtaining analytical results for other baths with modes in finite-dimensional spaces, such as spins other than $\frac{1}{2}$; we have not explored this possibility.

For the bosonic spin bath, the calculation is in the space of a single harmonic oscillator. It can be carried out by using operator identities.[1,2] We have used instead a method based on the coherent-state formalism which is detailed in the next section.

3. Exact Solution for the Density Matrix

We utilize the coherent-state formalism, e.g., Refs. 35, 36. The coherent states $|z\rangle$ are the eigenstates of the annihilation operator a with complex eigenvalues z. Note that from now on we omit the oscillator index k whenever this leads to no confusion. These states are not orthogonal:

$$\langle z_1|z_2\rangle = \exp\left(z_1^* z_2 - \frac{1}{2}|z_1|^2 - \frac{1}{2}|z_2|^2\right). \tag{3.1}$$

They form an over-complete set, and one can show that the identity operator in a single-oscillator space can be obtained as the integral

$$\int d^2 z\, |z\rangle\langle z| = 1\,. \tag{3.2}$$

Here the integration by definition corresponds to

$$d^2 z \equiv \frac{1}{\pi} d\,(\mathrm{Re}z)\, d\,(\mathrm{Im}z)\ . \tag{3.3}$$

Furthermore, for an arbitrary operator A, we have, in a single-oscillator space,

$$\mathrm{Tr}A = \int d^2z \, \langle z|A|z\rangle \, . \tag{3.4}$$

Finally, we note the following identity,[35] which will be used later,

$$e^{\Omega a^\dagger a} = \mathcal{N}\left[e^{a^\dagger(e^\Omega - 1)a}\right] . \tag{3.5}$$

In this relation Ω is an arbitrary c-number, while $\mathcal{N}$ denotes normal ordering.

The result (2.17) for the reduced density matrix, assuming the bosonic spin bath, can be written as

$$\rho_{mn}(t) = \rho_{mn}(0)e^{i(E_n - E_m)t}\prod_k S_{mn,k} \equiv [\rho_{mn}(t)]_{g_k=0}\prod_k S_{mn,k} \, , \tag{3.6}$$

where we used (2.9). Omitting the mode index k for simplicity, the expression for S_{mn} for each mode in the product is

$$S_{mn} = Z^{-1}\mathrm{Tr}\left[e^{-it\gamma_m}e^{-\beta\omega a^\dagger a}e^{it\gamma_n}\right] , \tag{3.7}$$

where the trace is in the space of that mode, and we defined

$$\gamma_m = \omega a^\dagger a + \lambda_m\left(g^* a + g a^\dagger\right) . \tag{3.8}$$

The partition function Z is given in (2.7). Relations (3.6)-(3.8) already illustrate one of our main results: apart from the phase factor which would be present in the noninteracting case anyway, the system energy eigenvalues E_n do not enter in the expression for $\rho_{mn}(t)$. The interesting time dependence is controlled by the eigenvalues λ_n of the "pointer observable" operator Λ_S (and by the heat-bath coupling parameters ω_k and g_k).

In order to evaluate the trace in (3.7), we use the coherent-state approach. We have

$$ZS_{mn} = \int d^2z_0\, d^2z_1\; d^2z_2\; \langle z_0|e^{-it\gamma_m}|z_1\rangle\langle z_1|e^{-\beta\omega a^\dagger a}|z_2\rangle\langle z_2|e^{it\gamma_n}|z_0\rangle\,. \tag{3.9}$$

The normal-ordering formula (3.5) then yields for the middle term,

$$\langle z_1|e^{-\beta\omega a^\dagger a}|z_2\rangle = \langle z_1|z_2\rangle e^{z_1^*(e^{-\beta\omega}-1)z_2} =$$

$$\exp\left[z_1^* z_2 - \frac{1}{2}|z_1|^2 - \frac{1}{2}|z_2|^2 + z_1^*(e^{-\beta\omega}-1)z_2\right]. \tag{3.10}$$

In order to evaluate the first and last factors in (3.9) we define shifted operators

$$\eta = a + \lambda_m \omega^{-1} g\,, \tag{3.11}$$

in terms of which we have

$$\gamma_m = \omega \eta^\dagger \eta - \lambda_m^2 \omega^{-1} |g|^2\,. \tag{3.12}$$

Since η and $\eta^\dagger$ still satisfy the bosonic commutation relation $[\eta, \eta^\dagger] = 1$, the normal-ordering formula applies. Thus, for the first factor in (3.9), for instance, we get

$$\langle z_0 | e^{-it\gamma_m} | z_1 \rangle = e^{it\lambda_m^2 \frac{|g|^2}{\omega}} \langle z_0 | z_1 \rangle e^{\left(e^{-i\omega t}-1\right)\left(z_0^* + \lambda_m \frac{g^*}{\omega}\right)\left(z_1 + \lambda_m \frac{g}{\omega}\right)}\,. \tag{3.13}$$

Collecting all these expressions, one concludes that the calculation of S_{mn} involves six Gaussian integrations over the real and imaginary parts of the variables z_0, z_1, z_2. This is a rather lengthy calculation but it can be carried out in closed form. The result, with indices k restored, is

$$S_{mn,k} = \exp\left(-\omega_k^{-2} |g_k|^2 P_{mn,k}\right)\,, \tag{3.14}$$

where

$$P_{mn,k} = 2\left(\lambda_m - \lambda_n\right)^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta\omega_k}{2} + i\left(\lambda_m^2 - \lambda_n^2\right)\left(\sin\omega_k t - \omega_k t\right) . \tag{3.15}$$

The expression (3.15), with (3.14), when inserted in (3.6), is the principal result of this section. It will be discussed in the next section. Here we note that in the studies of systems involving the bosonic heat bath one frequently adds the "renormalization" term[2,29] in the Hamiltonian,

$$H = H_S + H_B + H_I + H_R\,, \tag{3.16}$$

where in our case

$$H_R = \Lambda_S^2 \sum_k \omega_k^{-1} |g_k|^2 . \tag{3.17}$$

The role of this renormalization has been reviewed in Ref. 29. Here we only notice that the sole effect of adding this term in our calculation is to modify the imaginary part of $P_{mn,k}$ which plays no role in our subsequent discussion. The modified expression is

$$P_{mn,k} = 2\left(\lambda_m - \lambda_n\right)^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta\omega_k}{2} + i\left(\lambda_m^2 - \lambda_n^2\right)\sin\omega_k t\,. \tag{3.18}$$

4. Continuum Limit and Discussion

The results of the preceding section, (3.6), (3.14), (3.15), can be conveniently discussed if we consider magnitudes of the matrix elements of the reduced density matrix $\rho(t)$. We have

$$|\rho_{mn}(t)| = |\rho_{mn}(0)| \exp\left[-\frac{1}{4}(\lambda_m - \lambda_n)^2 \Gamma(t)\right], \tag{4.1}$$

where we introduced the factor $\frac{1}{4}$ to have the expression identical to that obtained in Ref. 14:

$$\Gamma(t) = 8 \sum_k \omega_k^{-2} |g_k|^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta \omega_k}{2}. \tag{4.2}$$

These results suggest several interesting conclusions. First, the decoherence is clearly controlled by the interaction with the heat bath rather than by the system's Hamiltonian. The eigenvalues of the "pointer observable" Λ_S determine the rate of decoherence, while the type of the bath and coupling controls the form of the function $\Gamma(t)$. It is interesting to note that states with equal eigenvalues λ_m will remain entangled even if their energies E_m are different. As expected, the magnitude of the diagonal matrix elements remains unchanged.

Secondly, we note that $\Gamma(t)$ is a sum of positive terms. However, for

true decoherence, i.e., in order for this sum to diverge for large times, one needs a continuum of frequencies and interactions with the bath modes that are strong enough at low frequencies; see below. From this point on, our discussion of the function $\Gamma(t)$ is basically identical to that in Ref. 14 (see also Ref. 1); we only outline the main points. In the continuum limit, exemplified for instance by phonon modes in solid state, we introduce the density of states $G(\omega)$ and sum over frequencies rather than modes characterized by their wave vectors. The latter change of the integration variable introduces the factor which we will loosely write as $\frac{dk}{d\omega}$; it must be calculated from the dispersion relation of the bosonic modes. Thus we have

$$\Gamma(t) \propto \int d\omega \, \frac{dk}{d\omega} G(\omega) |g(\omega)|^2 \, \omega^{-2} \sin^2 \frac{\omega t}{2} \coth \frac{\beta\omega}{2} \, . \tag{4.3}$$

In Ref. 14, the following choice was considered, motivated by properties of the phonon field in solids; see also Refs. 8-11, 12-18, 29:

$$\frac{dk}{d\omega} G(\omega) |g(\omega)|^2 \propto \omega^n e^{-\frac{\omega}{\omega_c}} \, . \tag{4.4}$$

This combination of the coupling constants and frequencies has been termed the spectral function. Here ω_c is the Debye cutoff frequency.

Specifically, the authors of Ref. 14 have analyzed the cases $n = 1$ and

$n = 3$. For $n = 1$, three regimes were identified, defined by the time scale for thermal decoherence, β, which is large for low temperatures, see (1.2), and the time scale for quantum-fluctuation effects, ω_c^{-1}. Recall that we use the units $\hbar = 1$. The present treatment only makes sense provided $\omega_c^{-1} \ll \beta$. According to Ref. 14, the first, "quiet" regime $t \ll \omega_c^{-1}$ corresponds to no significant decoherence and $\Gamma \propto (\omega_c t)^2$. The next, "quantum" regime, $\omega_c^{-1} \ll t \ll \beta$, corresponds to decoherence driven by quantum fluctuations and $\Gamma \propto \ln(\omega_c t)$. Finally, for $t \gg \beta$, in the "thermal" regime, thermal fluctuations play major role in decoherence and $\Gamma \propto t/\beta$.

For $n = 3$, decoherence is incomplete.[14] Indeed, while n must be positive for the integral in (4.3) to converge, only for $n < 2$ we have divergent $\Gamma(t)$ growing according to a power law for large times (in fact, $\propto t^{2-n}$) in the "thermal" regime. Thus, strong enough coupling $|g(\omega)|$ to the low-frequency modes of the heat bath is crucial for full decoherence.

In summary, we derived exact results for the model of decoherence due to energy-conserving interactions with the bosonic heat bath. We find that the spectrum of the "pointer observable" that enters the interaction with the bath controls the rate of decoherence. The precise functional form of the time dependence is determined both by the choice of heat-bath and system-bath coupling. However, for the case studied, it is universal

for all pointer observables and for all the matrix elements of the reduced density matrix.

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5.0 RESEARCH ARTICLE

Lower bounds for dechoherence

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ABSTRACT

Both quantum computing and tests of certain theories of quantum measurement require tight control over entanglement of the degrees of freedom of the system with those of the environment. In particular, one wishes to avoid entanglement-induced decoherence due to the confining of the system by the macroscopic apparatus. Nonetheless, when the system interacts with its walls (treated quantum mechanically), there is an inevitable intertwining of degrees of freedom. We show that *this need not lead to entanglement*, hence decoherence. It *will* generally lead to error. The wave function optimization required to avoid decoherence is also examined.

Keywords: Quantum computing, Analog computing, fundamental limits, experimental tests of quantum mechanics

1. INTRODUCTION

Practically speaking, the builder of a quantum computer has two difficult jobs: making sure the system stays in its own Hilbert space and making sure it is at the right location in that Hilbert space. The first of these is the problem of decoherence, the desire to avoid entanglement of system degrees of freedom with those of the apparatus holding and controlling the system. The second I call the problem of "error" (although others use this term differently), meaning there is no entanglement, but you just don't get the result intended.

The decoherence resulting from entanglement has significance beyond its importance for quantum computers: it has long been considered an essential ingredient in "quantum measurement." For example, when one wants to go from a quantum description to a master equation description of a system, the important step is a projection over background or environmental degrees of freedom. Because these environmental degrees of freedom have become entangled with the system, the projection causes the states characterized by different master equation labels to decohere from one another. When one gets to a yet more macroscopic level, Schrödinger cats and whatnot, the conceptual conundrums grow. For some people it's the ensembles that proliferate, for others it's worlds. In any case, the separation of the worlds or the use of ordinary probabilities in the ensembles, depend on entanglement-driven decoherence.[1]

It is not surprising then that the goals one has in trying to understand the quantum measurement process and in trying to build a quantum computer have a lot in common. In the oldest quantum measurement discussions one contemplated a separation between classical and quantum worlds. Atoms—governed by quantum mechanics—were 10^{-8} cm in size, and apparatus—governed by classical mechanics—was at least 10^{-4} cm. The state of technology did not challenge this separation of scales. Of course at the theoretical level no one was too happy with this view but it allowed people to treat the measurement process as somehow outside the usual Schrödinger (or Dirac, etc.) time evolution. Today this position can no longer be maintained. People have brought a detailed quantum description to larger and larger distance scales. Two systematic views of the measurement process that stick to ordinary quantum evolution throughout are the many-world interpretation and its outgrowths[2] and my own description,[3] which differs from the others in its treatment of the foundations of statistical mechanics. The main conceptual difference between these theories is that the many-world post-Everett view continues to maintain that from given initial conditions many outcomes are possible (and you cannot predict which will occur), while in my theory only one macroscopic outcome is possible. But the truly important difference is that if my ideas are correct there is the possibility of *experimental* differences from previous understandings of the measurement process, while the post-Everett ideas only reproduce (according to their advocates) the same physical predictions as the Copenhagen interpretation. (Notice that I distinguish between the laws of dynamics (Schrödinger's equation, etc.) and the way in which the evolved state is "measured" at the macroscopic level. For the first, Copenhagen, Everett, post-Everett and I agree. It is the second area where disagreement sets in.)

Granted then that technology has overtaken earlier ideas, how could this technology be used to elucidate the old problems? It is clear that one could put the old ideas to the test by *not* allowing a "measurement," by taking rather large systems, large enough to be considered apparatus, and having so much control over their detailed time evolution that the black magic of the measurement process could not operate. Such control is precisely the goal of the constructor of the quantum computer. Only pure unitary quantum evolution is supposed to take place, and of course the goal is to have this be true for systems of many components, the number of those components corresponding to the large integer associated with the size of the quantum computation (e.g., the number of digits in the number to be factored).

Suppose then that you've successfully built this "computer." It's big enough for the old measurement ideas to demand ensembles and such, but controlled enough so you don't invoke those ideas except perhaps at the final stage of the computation. Does this contrast have experimental consequences? For those[4] who propose that deviations from standard quantum evolution solve the measurement problem, indeed there should be such consequences. For variations on the many-worlds view it would seem (as indicated above) that there should be no experimental difference from what you'd get by talking about ensembles. On the other hand, for my understanding of the measurement process it is quite likely that experimental differences can be found. For me this has been the principal attraction of the flood of developments in quantum computing, especially at the experimental level.

In my forthcoming book, [3], is an elaboration of ways in which maintaining a large but "unmeasured" system could be used to test the validity of my own theories. The general principle is to produce a measurement situation but to eliminate the possibility of having what I call special states, thereby preventing some of the expected experimental outcomes. The absence of these otherwise expected outcomes would constitute the test of my theory. For example, suppose the system is under exquisite control (i.e., it does not entangle with its surroundings, including the walls confining it), but is sufficiently complex to itself function as a measurement apparatus. For example it might be a spin system of the sort contemplated in Ref. [5]. If a further level of "exquisite control" is possible, namely the prevention of a class of special states, then the possible outcomes of the time evolution would be different from that predicted by the usual quantum measurement theory. In this way one would have an experimental test of the theories of Ref. [3]. This is not the place for further elaboration and I refer the reader to that reference, which should appear shortly.

What emerges from these considerations is that both for the problem of quantum computation and for the testing of fundamental theories the avoidance of entanglement is paramount, as is the ability to control (or at least know) just where in Hilbert space the system is.

For this reason, I undertake in this article to examine a process that is ubiquitous in any macro/micro interface. Laboratory systems are pinned to the table. Even if your "system" is held in a electromagnetic trap, still the fields generating the trap are produced by apparatus standing on the floor. Just keeping a system in place means that from time-to-time it interacts with its confining walls, whatever they be. These "walls" must ultimately be treated as quantum systems. My question is, will the small-system degrees of freedom become entangled with the wall degrees of freedom? I expect this effect to be small, but as a matter of principle, I ask whether there must always be such entanglement?

As a form of system-container interaction I take the system to be confined within hard walls. This means that when the system or a part of it does interact with its container it does so by means of a scattering that can be more or less localized in time. Starting from this assumption I take the approach in [6]. We begin from the inevitable post-collision intertwining of wall and system, and establish the extent to which it leads to entanglement. The measure of entanglement is that given in [7].

It turns out that there is a surprise: for appropriately tailored wave functions, there need be no decoherence! This leads us to explore the significance of the tailoring. However, although *decoherence* is avoidable, we will show that *error* is not.[8]

For studies of quantum computing, one must also bear in mind that whether the decoherence is large or small (for nearly matching wave functions it is of order system/container mass ratio) the resulting amplitude defect must be subtracted from the wave function for *each* collision. This may lead to physically significant effects.

2. INTERACTING WITH A WALL

As indicated, we assume that the system will, from time to time, collide with its container. Dissipative walls (i.e., inelastic collisions) immediately lead to entanglement; we therefore assume that the collision is elastic and involves no degree of freedom beyond that required to contain the system. Our model is thus the scattering of two point particles, one of mass m (small) representing the microscopic system, and one of mass M (large), representing the container.[9]

Before the collision we assume the wave function to be $\Psi_I = \Gamma(X)\Phi(x)$ (hence unentangled), with position variables X and x corresponding to the large and small masses, respectively. We make several assumptions: 1.) Restriction to one dimension, reasonable if the large "particle" is in fact a wall. 2.) Rapid completion of the scattering. 3) Short range, infinite repulsion. 4.) Gaussian wave packets. Assumptions #2 and #3 are reasonable and simplify the calculation, and I expect departures from them to increase decoherence and error.

If the interaction with the wall could be treated as a pure potential-interaction with a fixed object, the wave function after the collision would be[10] $\Gamma(X)\Phi(-x)$. On the other hand, the correct form of the final wave function can be seen by going to center of mass coordinates, $R = (MX + mx)/\mathcal{M}$, $u = x - X$, with $\mathcal{M} = M + m$. In these coordinates $\Psi_I = \Gamma(R - \delta u)\Phi(R + \gamma u)$, where $\delta = m/\mathcal{M}$ and $\gamma = M/\mathcal{M}$. With the above assumptions, the wave function *after* the collision is $\Psi_F = \Gamma(R+\delta u)\Phi(R-\gamma u)$, i.e., $u \to -u$. To show this, recall that the exact propagator for this problem is

$$G(R'', u'', t; R', u') = g_0^M(R'' - R', t)\,[g_0^m(u'' - u', t) - g_0^m(u'' + u', t)]$$

with

$$g_0^\mu(y,t) \equiv \sqrt{\frac{\mu}{2\pi i\hbar t}}\exp\left(\frac{i\mu y^2}{2t\hbar}\right) .$$

the free propagator. To a good approximation, before the collision the wave function is given by the integral involving $g_0^m(u'' - u', t)$, after the collision by that involving $g_0^m(u'' + u', t)$. Thus to get the final wave function, one reverses "u".

When re-expressed in terms of x and X, $\Psi_F = \Gamma(X(1-2\delta)+2x\delta)\Phi(-x(1-2\delta)+2X\gamma)$, suggesting that the final wave function has become entangled. For interactions more general than the hard wall there will be more complicated changes in the functions, but since the separate evolution of u and R follows from momentum conservation and the general nature of the two-particle interaction, there is no getting away from the intertwining.

The form we take for the wave function is

$$\Psi_I = \frac{1}{\sqrt{2\pi\sigma\Sigma}}\exp\left(-\frac{X^2}{4\Sigma^2}\right)\exp\left(-\frac{x^2}{4\sigma^2} + ikx\right) \tag{1}$$

with both x and X taking values on the entire real line. The position spreads are $\Delta X = \Sigma$ and $\Delta x = \sigma$, both assumed real. In principle we should use a wave function with "$x - x_0$" in place of "x" above and restrict the relative coordinate to (say) negative values (because of the hard wall). However, the form of the propagator given above allows us to use the simpler form, Eq. (1). That propagator says that one can look upon this scattering as taking place on the entire line but with a second source at a reflected position (this is the method of images applied to the path integral). The wave emanating from the image is the wave function for large positive times, and this is the portion we wish to study. In particular we look at its inner product with a test wave function (what you would have taken to be the wave function had you not treated the wall as a quantum dynamical object) and study its entanglement properties using the measure of [7]. However, the answer to neither of these questions will change with time so that we can study the reflected wave at whatever time is most convenient and, as in Eq. (1), that time is the time for which there is symmetry in x. However, since this is now to be thought of as the reflected wave moved back to an earlier time, the *entire* reflected wave must be used, i.e., variables range over the entire line. Although this trick is available only when the method of images can be applied, the general tenor of our results does not depend on it. You can (also in this case) start the wave packet at some (say, negative) x_0 and propagate it through the impact. The only thing to be careful of (which also applies to our argument above) is that the incoming and outgoing waves separate on a time scale less than that for wave packet spreading.

We now check error and decoherence. To compute "error," we compare the outgoing wave to the final state had the wall not been treated dynamically. To compute decoherence we measure the degree of entanglement as defined in [7].

3. ERROR

We examine the overlap integral of the actual Ψ_F with the wave function that would have resulted from the idealization, $x \to -x$, namely $\Psi_{\rm test} \equiv \Gamma(X)\Phi(-x) = \Gamma(R-\delta u)\Phi(-R-\gamma u)$. Using Eq. (1)

$$\begin{aligned} A &\equiv \int \Psi^*_{\rm test}\Psi_F = \int dRdu\Gamma^*(R-\delta u)\Phi^*(-R-\gamma u)\Gamma(R+\delta u)\Phi(R-\gamma u) \\ &= \frac{1}{2\pi\sigma\Sigma}\int dRdu \exp\left(-\frac{(R-\delta u)^2}{4\Sigma^2} - \frac{(-R-\gamma u)^2}{4\sigma^2} - ik(-R-\gamma u)\right) \\ &\quad \times \exp\left(-\frac{(R+\delta u)^2}{4\Sigma^2} - \frac{(R-\gamma u)^2}{4\sigma^2} + ik(R-\gamma u)\right) \end{aligned}$$

We find

$$A^{-2} = \left[\gamma^2 + \delta^2 + \gamma^2\lambda + \frac{\delta^2}{\lambda}\right]\exp\left(\frac{4k^2\lambda\sigma^2}{1+\lambda}\right) \qquad \text{with } \lambda \equiv \frac{\Sigma^2}{\sigma^2} \tag{2}$$

Particular experiments have their own particular wave functions; hence A's deviation from 1 varies. Here we vary σ and Σ so as to minimize the deviation (and maximize A). Of course this option may not be open to an experimentalist and our calculation represents the best one could obtain. For $k = 0$, A depends only on λ (not the sigmas separately), and is optimized by

$$\lambda_{\rm max} = \frac{\delta}{\gamma} \approx \frac{m}{M}$$

Substituting yields $A = 1$. There is *no* error! (N.B., ... *only* for $\lambda = \lambda_{\rm max}$.) When $k \neq 0$ we maximize A by optimizing λ for given $k\sigma$. We will see that even at best A falls below unity by $O(\delta)$. For small and large $k\sigma$ analytic forms are

Small $k\sigma$	$\lambda_{\rm max} \approx \delta/\gamma$ (as before)	$1 - A \approx 2\delta k^2\sigma^2$
Large $k\sigma$	$\lambda_{\rm max} \approx \delta/2k\sigma$	$1 - A \approx 2\delta k\sigma$

(3)

These behaviors mesh smoothly at $k\sigma \sim 1$. Eq. (3) is a lower bound on error. Again, we recall that this is a mathematical result; it may not be possible to realize in the laboratory. The factor $\delta \approx m/M$ keeps this effect small and is reminiscent of similar factors in measurement theory.[11] It may be appropriate to think of the confinement process as one in which the system's components are constantly bumping up against their container, so that the small δ could pick up a large factor related to an effective frequency of such interactions.

4. DECOHERENCE

This is potentially the more damaging effect. A basis independent measure of the degree of entanglement of the particle and wall is given in [7]. It can be shown that this degree of entanglement is 1 minus the largest eigenvalue of $\psi^\dagger\psi$ (or $\psi\psi^\dagger$) considered as a matrix operator with matrix indices the arguments of ψ.

Because we ultimately wish to use the system variable x as if it were unentangled, the wave function is expressed in terms of x and X:

$$\begin{aligned} \Psi_F(x,X) = \left(\frac{4\Omega\omega}{\pi^2}\right)^{1/4} \exp\Big\{&-\Omega\left[X(1-2\delta) + 2\delta x\right]^2 - \omega\left[x(1-2\gamma) + 2\gamma X\right]^2 \\ &+ ik\left[x(1-2\gamma) + 2\gamma X\right]\Big\} \end{aligned} \tag{4}$$

with $\Omega \equiv 1/4\Sigma^2$, and $\omega \equiv 1/4\sigma^2$. We can form an operator either by integrating over X or over x. We choose

$$\begin{aligned} F(x',x) &\equiv \int dX \Psi_F^*(X,x')\Psi_F(X,x) \\ &= \sqrt{\frac{2\omega\Omega}{\pi D}} \exp\left\{-(x^2+x'^2)\frac{\omega\Omega}{D} - (x-x')^2\frac{E^2}{D} + ik(1-2\gamma)(x-x')\right\} \end{aligned} \tag{5}$$

with $D \equiv \Omega(\gamma-\delta)^2 + 4\omega\gamma^2$, and $\rho \equiv |(\gamma-\delta)(\Omega\delta - \omega\gamma)|$. As indicated, we want the largest eigenvalue of F, now thought of as the integral kernel of an operator. Note that the factor $\exp[ik(1-2\gamma)(x-x')]$ can be dropped because it does not affect the eigenvalue. Next observe that F is almost the same as the kernel of the propagator for the simple harmonic oscillator. Using a standard form for this operator,[12] we can immediately deduce information about eigenvalues. The operator

$$G(x,y) \equiv \sqrt{\frac{\beta}{\pi \sinh u}} \exp\left[-\frac{\beta}{\sinh u}\left[(x^2+y^2)\cosh u - 2xy\right]\right]$$

has the spectrum $G_n = \exp[-u(n+1/2)]$, $n = 0,1,2,\ldots$, irrespective of β. (The connection with the oscillator is $\beta = m\omega/2\hbar$ and $\omega t = -iu$.) It is now straightforward to deduce that the spectrum of F is $F_n = (1-e^{-u})e^{-nu}$, with $n = 0,1,\ldots$, and $\sinh u/2 = \sqrt{\omega\Omega}/2\rho$. It follows that the largest eigenvalue of F is

$$F_0 = 1 - z^2 \ , \text{ with } \ z = \sqrt{\frac{w^2}{4}+1} - \frac{w}{2} \ , \ \text{ and } w \equiv \frac{\sqrt{\omega\Omega}}{\rho}$$

For small w, $F_0 \sim w$, and for large w, $F_0 \sim 1 - 1/w^2$.

The first issue is minimizing entanglement, that is maximizing F_0. Clearly F_0 reaches its theoretical maximum for $w = \infty$, which requires in turn $\Omega\delta = \omega\gamma$. Recalling the definitions of ω and Ω this brings us to the same relation, $\Sigma^2/\sigma^2 = \delta/\gamma$, that we found when minimizing error.[13] It is interesting that here the entanglement is strictly zero *even when the momentum, k, is non-zero*—if there is the special matching of wave function spreads. In the absence of matching, the entanglement, hence the decoherence, can be considerable, as indicated by $F_0 \sim w$ for small w.

This decoherence cuts down the *amplitude* of the wave function that can ultimately yield an accurate computational result. By the methods of [7] one can show that the maximum amplitude available in a putative unentangled wave function $\psi(x)$ is $\sqrt{F_0}$ and that for two successive independent collisions it will be the product of two such terms. If F_0 is not extremely close to 1, the effect can build rapidly. Such behavior is to be contrasted with say, decay, where the initial small deviation is in a phase, so that the effect of many independent such deviations is only quadratic in each of them.

5. OPTIMAL COHERENCE

The minimization of both error and entanglement have brought to light a matching condition on the spreads of the system and apparatus, $\Sigma^2/\sigma^2 = m/M$. This may be surprising. Based on the usual idealization of macroscopic objects, one might have thought that there should be no restriction on the *smallness* of "ΔX".[14] Aside from considerations of the sort in [3] (and for which $F_0 = 1$ provides an example of a "special state"), there is no reason to think that Nature would evolve into minimally decohering states.[15] Of course the constructor of a quantum computer may have a strong interest in such minimizing. In any case it is of interest to consider the possibility that the optimizing condition hold generally. In [6] it was observed that *all* pairs of objects could satisfy the relation above if for each object, its mass, μ, and its position uncertainty, σ_μ, were related by $\sigma_\mu^2 \sim 1/\mu$. Possible justifications were considered in [6], but we here take the relation as a hypothesis and extend it using dimensional analysis.[16] Taking $\hbar = 1$ and $c = 1$, it is clear that another length (or energy or mass) is needed. For a confined system the quantities that come to mind are an overall distance scale for the system and the temperature. The former seems to me ill defined, and in particular an attractive feature of the relation proposed is that it is not vital to distinguish between "system" and walls. Using then the temperature (T) and restoring $\hbar$, we find

$$\sigma_\mu^2 \sim \frac{\hbar^2}{\mu k_B T} \tag{6}$$

with k_B the Boltzmann constant. Eq. (6) gives a mass-μ object a packet size that is the geometric mean of its Compton wavelength and $\sim 0.2\,\mathrm{cm}/T$ kelvins. This does not seem inconsistent with experience. Lower temperature allows larger coherent wave packets, distinguishing this effect from thermal fluctuations[17] where position spread *decreases* with decreasing temperature. If the effective momentum, k, of the small mass is itself the result of thermal fluctuations, then equipartition relates this to temperature as well. We then have $k^2\sigma^2 \sim (2\hbar^2k^2/2\mu)/k_BT \sim 1$, independent of temperature. (For $k\sigma = 1$, $A \approx 1 - 1.2\,\delta$.) This suggests that in a heat bath, $\Delta p \sim \hbar/\Delta x$, since $\langle p \rangle = 0$.

6. LIMITATIONS AND EXTENSIONS

We have shown that confinement need *not* force entanglement. This is good news for the program of testing the theories of Ref. [3], where entanglement may be an even more serious obstacle than it is in quantum computing. On the other hand, if the confined objects strike the walls at finite velocity, there must be "error." It must be emphasized that the no-entanglement result depends not only on a particular ratio of spreads for small and large system, but also on the Gaussian form of the wave packet and on the form of the interaction with the wall. We have not here explored the effect of relaxing these assumptions. Minimizing error relies on the same framework, so that one could entertain the idea of reducing error through tailoring of the wave packet or the walls. Based on preliminary exploration, I would say that more complicated wave packets or walls only increase both entanglement and error.

For applications it is desirable to identify the wall mass, "M". Even for a vacuum chamber one would not look to the mass of the entire chamber, but only the region affected by the particle's collision, perhaps defined by the wavelength of the appropriate phonon. For "chambers" that are magnetic fields (etc.) one can ultimately look to the laboratory equipment that produces these fields.

Finally, there is our decoherence-minimizing relation, $\sigma_\mu^2 \sim 1/\mu$, or more ambitiously, $\sigma_\mu^2 \sim \hbar^2/\mu k_B T$. Do particles settle into wave packets of this size? Are two-time boundary condition considerations (as in [3]) at work? Or perhaps (not exclusively) arguments of the form in [6] or [15] hold. Yet another question is the form such a relation might take for massless particles. Here too one could ask for decoherence-minimizing scattering.

In conclusion, we have shown that pinning a system to the table does not in itself force entanglement with the degrees of freedom of the container—treating the latter as a fully quantum object. Nevertheless, subject to reasonable assumptions, that pinning will introduce "error," in the sense of changed outgoing wave function. Minimizing both decoherence and error are best accomplished when a particular relation exists between the wave function spreads of system and container. We have also computed the degree of entanglement in situations where the minimum spread condition does not hold.

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8. By "decoherence" I mean loss of the primary wave function through entanglement with other degrees of freedom, hence the inability to interfere with portions of the wave function not so entangled. By "error" I mean non-entangled wave function whose value is changed from that in the absence of the scattering.
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14. There is of course Feynman's variation on the two slit experiment (in R. P. Feynman, R. B. Leighton and M. Sands, *The Feynman Lectures on Physics*, Addison-Wesley, Reading, MA (1965)), which relates uncertainties in a macroscopic object to putative measurements of a microscopic one. The corresponding restriction here would be that ΔX $(= \Sigma)$ not be so small that the associated ΔP destroy the small-system interference patterns that we seek. Our optimal Σ is far from such values. We estimate this kinematic effect as follows. Momentum uncertainty ΔP in the big system means uncertainty $\Delta P/M$ in the (velocity) transformation going into the center of mass frame. For the small system this velocity uncertainty gives a momentum uncertainty $(\Delta p)' \sim m(\Delta P/M)$ (the prime on $(\Delta p)'$ distinguishes it from the momentum uncertainty in the original wave function, namely $(\Delta p)_{\rm usual} \sim \hbar/\sigma$). Taking $\Delta P \sim \hbar/\Sigma$, we find $(\Delta p)' \sim m\hbar/M\Sigma$. Using $\Sigma^2/\sigma^2 \approx m/M$ yields $(\Delta p)'/(\Delta p)_{\rm usual} \sim \sqrt{m/M}$.
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